```
REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.65 A
REMARK starting r= 0.2072 free_r= 0.2361
REMARK final    r= 0.2072 free_r= 0.2361
REMARK B rmsd for bonded mainchain atoms= 1.427  target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.420  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.189  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.637  target= 2.5
REMARK rweight=  0.1000 (with wa= 0.987736)
REMARK target= mlf  steps= 30
REMARK sg= P1 a= 41.23 b= 65.22 c= 73.38 alpha= 73.11 beta= 85.58 gamma= 85.8
REMARK parameter file 1   : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2   : CNS_TOPPAR:water_rep.param
REMARK molecular structure file: amy.mtf
REMARK input coordinates: amy.pdb
REMARK reflection file= amy.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.65
REMARK initial B-factor correction applied to fobs :
REMARK    B11= -3.662 B22=  2.485 B33=  1.177
REMARK    B12=  2.042 B13=  2.748 B23=  -0.502
REMARK B-factor correction applied to coordinate array B:     0.012
REMARK bulk solvent: density level= 0.36444 e/A^3, B-factor= 46.0136 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range:   87646 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):  2854 (   3.3 % )
REMARK number of reflections rejected:                           0 (   0.0 % )
REMARK total number of reflections used:                     84792 (  96.7 % )
REMARK number of reflections in working set:                 80566 (  91.9 % )
REMARK number of reflections in test set:                     4226 (   4.8 % )
CRYST1   41.230   65.220   73.380  73.11  85.58  85.80 P 1
REMARK FILENAME="/work/olieric/db/db2-5_P1/cns/bindividual.pdb"
REMARK DATE:31-Mar-03  11:57:01       created by user: olieric
REMARK VERSION:1.1
ATOM      1  CB  MET A   1     -14.276 -31.220  16.788  1.00 17.29      A
ATOM      2  CG  MET A   1     -13.562 -30.976  15.453  1.00 19.06      A
ATOM      3  SD  MET A   1     -13.791 -29.325  14.750  1.00 20.01      A
ATOM      4  CE  MET A   1     -12.595 -28.385  15.663  1.00 20.04      A
ATOM      5  C   MET A   1     -12.346 -32.264  17.931  1.00 17.38      A
ATOM      6  O   MET A   1     -12.094 -31.451  18.823  1.00 18.05      A
ATOM      7  N   MET A   1     -14.641 -32.810  18.672  1.00 17.69      A
ATOM      8  CA  MET A   1     -13.789 -32.489  17.479  1.00 17.26      A
ATOM      9  N   LYS A   2     -11.404 -32.959  17.305  1.00 16.63      A
ATOM     10  CA  LYS A   2      -9.991 -32.827  17.687  1.00 17.10      A
ATOM     11  CB  LYS A   2      -9.686 -33.813  18.819  1.00 20.78      A
ATOM     12  CG  LYS A   2      -8.255 -33.915  19.217  1.00 24.62      A
ATOM     13  CD  LYS A   2      -8.095 -34.972  20.295  1.00 28.83      A
ATOM     14  CE  LYS A   2      -6.710 -34.905  20.918  1.00 31.65      A
ATOM     15  NZ  LYS A   2      -6.617 -35.825  22.100  1.00 33.43      A
ATOM     16  C   LYS A   2      -9.119 -33.168  16.483  1.00 17.18      A
ATOM     17  O   LYS A   2      -9.455 -34.064  15.706  1.00 14.51      A
ATOM     18  N   PHE A   3      -8.034 -32.423  16.284  1.00 14.64      A
ATOM     19  CA  PHE A   3      -7.135 -32.762  15.187  1.00 14.50      A
ATOM     20  CB  PHE A   3      -7.652 -32.265  13.810  1.00 16.07      A
ATOM     21  CG  PHE A   3      -7.818 -30.761  13.686  1.00 15.16      A
ATOM     22  CD1 PHE A   3      -9.067 -30.157  13.880  1.00 15.68      A
ATOM     23  CD2 PHE A   3      -6.737 -29.955  13.299  1.00 12.43      A
ATOM     24  CE1 PHE A   3      -9.233 -28.776  13.690  1.00 15.69      A
ATOM     25  CE2 PHE A   3      -6.888 -28.598  13.109  1.00 15.35      A
ATOM     26  CZ  PHE A   3      -8.163 -27.996  13.313  1.00 14.58      A
ATOM     27  C   PHE A   3      -5.783 -32.146  15.480  1.00 15.40      A
ATOM     28  O   PHE A   3      -5.685 -31.234  16.283  1.00 14.89      A
ATOM     29  N   THR A   4      -4.732 -32.697  14.884  1.00 13.77      A
ATOM     30  CA  THR A   4      -3.407 -32.124  15.046  1.00 15.62      A
ATOM     31  CB  THR A   4      -2.486 -32.956  15.948  1.00 17.56      A
ATOM     32  OG1 THR A   4      -3.030 -32.988  17.274  1.00 18.68      A
ATOM     33  CG2 THR A   4      -1.084 -32.288  16.013  1.00 18.01      A
ATOM     34  C   THR A   4      -2.846 -32.111  13.645  1.00 15.42      A
ATOM     35  O   THR A   4      -2.880 -33.120  12.942  1.00 17.97      A
ATOM     36  N   VAL A   5      -2.317 -30.970  13.238  1.00 16.55      A
ATOM     37  CA  VAL A   5      -1.804 -30.886  11.883  1.00 16.64      A
ATOM     38  CB  VAL A   5      -2.948 -30.508  10.930  1.00 18.41      A
ATOM     39  CG1 VAL A   5      -3.416 -29.040  11.181  1.00 18.38      A
ATOM     40  CG2 VAL A   5      -2.514 -30.773   9.468  1.00 19.99      A
ATOM     41  C   VAL A   5      -0.679 -29.886  11.773  1.00 17.93      A
ATOM     42  O   VAL A   5      -0.559 -28.960  12.592  1.00 16.18      A
ATOM     43  N   GLU A   6       0.166 -30.070  10.765  1.00 16.71      A
ATOM     44  CA  GLU A   6       1.253 -29.120  10.579  1.00 18.01      A
ATOM     45  CB  GLU A   6       2.218 -29.605   9.499  1.00 19.85      A
ATOM     46  CG  GLU A   6       3.012 -30.850   9.875  1.00 24.39      A
ATOM     47  CD  GLU A   6       3.999 -31.273   8.780  1.00 30.54      A
ATOM     48  OE1 GLU A   6       4.475 -30.396   8.006  1.00 30.19      A
ATOM     49  OE2 GLU A   6       4.317 -32.484   8.709  1.00 31.65      A
ATOM     50  C   GLU A   6       0.734 -27.751  10.164  1.00 17.50      A
ATOM     51  O   GLU A   6      -0.166 -27.642   9.334  1.00 17.39      A
ATOM     52  N   ARG A   7       1.337 -26.703  10.717  1.00 15.98      A
ATOM     53  CA  ARG A   7       0.975 -25.341  10.359  1.00 16.73      A
ATOM     54  CB  ARG A   7       1.539 -24.375  11.051  1.00 16.92      A
ATOM     55  CG  ARG A   7       1.902 -22.950  10.542  1.00 15.16      A
ATOM     56  CD  ARG A   7       3.010 -22.130  11.223  1.00 15.81      A
ATOM     57  NE  ARG A   7       3.117 -20.745  10.778  1.00 16.48      A
ATOM     58  CZ  ARG A   7       3.906 -20.342   9.787  1.00 19.48      A
ATOM     59  NH1 ARG A   7       4.650 -21.243   9.135  1.00 19.10      A
ATOM     60  NH2 ARG A   7       3.953 -19.063   9.445  1.00 19.15      A
ATOM     61  C   ARG A   7       1.077 -25.168   8.842  1.00 19.33      A
ATOM     62  O   ARG A   7       0.232 -24.536   8.201  1.00 20.23      A
ATOM     63  N   GLU A   8       2.116 -25.777   8.284  1.00 20.57      A
ATOM     64  CA  GLU A   8       2.392 -25.680   6.869  1.00 23.30      A
ATOM     65  CB  GLU A   8       3.669 -26.474   6.585  1.00 25.23      A
```

Figure 1 (1)

ATOM	66	CG	GLU	A	8	4.958	-25.909	7.259	1.00	29.45	A
ATOM	67	CD	GLU	A	8	4.840	-25.478	8.733	1.00	28.90	A
ATOM	68	OE1	GLU	A	8	4.512	-26.346	9.633	1.00	28.78	A
ATOM	69	OE2	GLU	A	8	5.119	-24.257	8.986	1.00	23.71	A
ATOM	70	C	GLU	A	8	1.213	-26.154	6.007	1.00	22.79	A
ATOM	71	O	GLU	A	8	0.997	-25.624	4.913	1.00	24.80	A
ATOM	72	N	HIS	A	9	0.433	-27.108	6.514	1.00	21.38	A
ATOM	73	CA	HIS	A	9	-0.711	-27.627	5.748	1.00	21.73	A
ATOM	74	CB	HIS	A	9	-1.034	-29.064	6.157	1.00	23.42	A
ATOM	75	CG	HIS	A	9	0.111	-30.021	6.010	1.00	27.55	A
ATOM	76	CD2	HIS	A	9	1.279	-29.926	5.335	1.00	29.37	A
ATOM	77	ND1	HIS	A	9	0.136	-31.242	6.644	1.00	27.98	A
ATOM	78	CE1	HIS	A	9	1.273	-31.856	6.376	1.00	28.44	A
ATOM	79	NE2	HIS	A	9	1.986	-31.080	5.583	1.00	30.06	A
ATOM	80	C	HIS	A	9	-1.974	-26.796	5.903	1.00	22.06	A
ATOM	81	O	HIS	A	9	-2.916	-26.941	5.113	1.00	20.93	A
ATOM	82	N	LEU	A	10	-2.007	-25.930	6.909	1.00	20.66	A
ATOM	83	CA	LEU	A	10	-3.169	-25.074	7.155	1.00	21.35	A
ATOM	84	CB	LEU	A	10	-3.366	-24.857	8.655	1.00	21.25	A
ATOM	85	CG	LEU	A	10	-4.041	-25.917	9.494	1.00	22.14	A
ATOM	86	CD1	LEU	A	10	-4.016	-25.491	10.958	1.00	22.44	A
ATOM	87	CD2	LEU	A	10	-5.499	-26.105	9.002	1.00	19.68	A
ATOM	88	C	LEU	A	10	-3.135	-23.695	6.547	1.00	22.26	A
ATOM	89	O	LEU	A	10	-4.182	-23.091	6.321	1.00	24.22	A
ATOM	90	N	LEU	A	11	-1.935	-23.173	6.349	1.00	22.98	A
ATOM	91	CA	LEU	A	11	-1.731	-21.819	5.853	1.00	25.99	A
ATOM	92	CB	LEU	A	11	-0.223	-21.587	5.647	1.00	27.18	A
ATOM	93	CG	LEU	A	11	0.489	-20.748	6.712	1.00	31.58	A
ATOM	94	CD1	LEU	A	11	-0.093	-20.987	8.066	1.00	31.86	A
ATOM	95	CD2	LEU	A	11	1.991	-21.058	6.673	1.00	31.87	A
ATOM	96	C	LEU	A	11	-2.497	-21.417	4.602	1.00	24.67	A
ATOM	97	O	LEU	A	11	-3.300	-20.487	4.638	1.00	24.80	A
ATOM	98	N	LYS	A	12	-2.270	-22.122	3.507	1.00	24.14	A
ATOM	99	CA	LYS	A	12	-2.949	-21.784	2.263	1.00	25.70	A
ATOM	100	CB	LYS	A	12	-2.393	-22.627	1.102	1.00	28.62	A
ATOM	101	CG	LYS	A	12	-2.758	-22.084	-0.282	1.00	33.62	A
ATOM	102	CD	LYS	A	12	-2.196	-22.974	-1.407	1.00	36.68	A
ATOM	103	CE	LYS	A	12	-3.036	-24.242	-1.643	1.00	39.26	A
ATOM	104	NZ	LYS	A	12	-3.304	-25.093	-0.433	1.00	38.98	A
ATOM	105	C	LYS	A	12	-4.458	-21.963	2.397	1.00	22.87	A
ATOM	106	O	LYS	A	12	-5.233	-21.072	2.031	1.00	24.13	A
ATOM	107	N	PRO	A	13	-4.906	-23.118	2.922	1.00	21.49	A
ATOM	108	CD	PRO	A	13	-4.218	-24.387	3.212	1.00	21.35	A
ATOM	109	CA	PRO	A	13	-6.359	-23.257	3.052	1.00	21.39	A
ATOM	110	CB	PRO	A	13	-6.521	-24.589	3.774	1.00	20.96	A
ATOM	111	CG	PRO	A	13	-5.337	-25.379	3.227	1.00	21.10	A
ATOM	112	C	PRO	A	13	-6.972	-22.103	3.836	1.00	20.93	A
ATOM	113	O	PRO	A	13	-7.985	-21.545	3.431	1.00	21.33	A
ATOM	114	N	LEU	A	14	-6.369	-21.735	4.967	1.00	21.72	A
ATOM	115	CA	LEU	A	14	-6.920	-20.646	5.762	1.00	22.99	A
ATOM	116	CB	LEU	A	14	-6.111	-20.432	7.048	1.00	22.66	A
ATOM	117	CG	LEU	A	14	-6.506	-21.332	8.208	1.00	19.80	A
ATOM	118	CD1	LEU	A	14	-5.520	-21.068	9.351	1.00	19.78	A
ATOM	119	CD2	LEU	A	14	-7.951	-21.053	8.667	1.00	19.15	A
ATOM	120	C	LEU	A	14	-6.992	-19.318	5.041	1.00	26.19	A
ATOM	121	O	LEU	A	14	-7.964	-18.577	5.189	1.00	27.05	A
ATOM	122	N	GLN	A	15	-5.947	-18.995	4.297	1.00	27.38	A
ATOM	123	CA	GLN	A	15	-5.935	-17.742	3.574	1.00	31.46	A
ATOM	124	CB	GLN	A	15	-4.608	-17.570	2.842	1.00	33.84	A
ATOM	125	CG	GLN	A	15	-4.472	-16.213	2.182	1.00	38.53	A
ATOM	126	CD	GLN	A	15	-3.117	-16.025	1.545	1.00	41.36	A
ATOM	127	OE1	GLN	A	15	-2.080	-16.062	2.223	1.00	42.71	A
ATOM	128	NE2	GLN	A	15	-3.109	-15.827	0.230	1.00	43.79	A
ATOM	129	C	GLN	A	15	-7.081	-17.731	2.568	1.00	32.51	A
ATOM	130	O	GLN	A	15	-7.813	-16.741	2.440	1.00	32.62	A
ATOM	131	N	GLN	A	16	-7.250	-18.852	1.878	1.00	32.52	A
ATOM	132	CA	GLN	A	16	-8.284	-18.960	0.862	1.00	33.60	A
ATOM	133	CB	GLN	A	16	-8.191	-20.314	0.161	1.00	34.74	A
ATOM	134	CG	GLN	A	16	-9.193	-20.486	-0.970	1.00	38.72	A
ATOM	135	CD	GLN	A	16	-8.630	-20.088	-2.328	1.00	41.86	A
ATOM	136	OE1	GLN	A	16	-8.139	-18.960	-2.519	1.00	42.92	A
ATOM	137	NE2	GLN	A	16	-8.701	-21.018	-3.286	1.00	41.57	A
ATOM	138	C	GLN	A	16	-9.698	-18.767	1.398	1.00	32.72	A
ATOM	139	O	GLN	A	16	-10.502	-18.042	0.808	1.00	33.73	A
ATOM	140	N	VAL	A	17	-10.018	-19.396	2.521	1.00	31.34	A
ATOM	141	CA	VAL	A	17	-11.371	-19.262	3.041	1.00	32.67	A
ATOM	142	CB	VAL	A	17	-11.801	-20.516	3.822	1.00	29.85	A
ATOM	143	CG1	VAL	A	17	-11.679	-21.733	2.928	1.00	28.35	A
ATOM	144	CG2	VAL	A	17	-10.948	-20.683	5.063	1.00	29.58	A
ATOM	145	C	VAL	A	17	-11.608	-18.045	3.917	1.00	35.48	A
ATOM	146	O	VAL	A	17	-12.757	-17.663	4.130	1.00	34.98	A
ATOM	147	N	SER	A	18	-10.539	-17.448	4.431	1.00	39.01	A
ATOM	148	CA	SER	A	18	-10.672	-16.274	5.294	1.00	43.39	A
ATOM	149	CB	SER	A	18	-9.520	-16.208	6.292	1.00	43.24	A
ATOM	150	OG	SER	A	18	-9.475	-17.366	7.099	1.00	44.08	A
ATOM	151	C	SER	A	18	-10.695	-14.990	4.477	1.00	46.76	A
ATOM	152	O	SER	A	18	-11.095	-13.932	4.982	1.00	46.88	A
ATOM	153	N	GLY	A	19	-10.266	-15.096	3.221	1.00	50.03	A
ATOM	154	CA	GLY	A	19	-10.221	-13.953	2.322	1.00	54.68	A
ATOM	155	C	GLY	A	19	-11.387	-12.985	2.438	1.00	57.76	A
ATOM	156	O	GLY	A	19	-11.234	-11.899	3.011	1.00	58.12	A
ATOM	157	N	PRO	A	20	-12.566	-13.333	1.893	1.00	60.08	A
ATOM	158	CD	PRO	A	20	-12.947	-14.603	1.250	1.00	60.71	A
ATOM	159	CA	PRO	A	20	-13.713	-12.425	1.989	1.00	62.25	A
ATOM	160	CB	PRO	A	20	-14.831	-13.208	1.289	1.00	62.05	A
ATOM	161	CG	PRO	A	20	-14.434	-14.648	1.497	1.00	61.28	A
ATOM	162	C	PRO	A	20	-14.040	-12.092	3.450	1.00	64.35	A
ATOM	163	O	PRO	A	20	-14.838	-12.786	4.088	1.00	64.86	A
ATOM	164	N	LEU	A	21	-13.420	-11.032	3.976	1.00	66.50	A
ATOM	165	CA	LEU	A	21	-13.636	-10.631	5.368	1.00	68.70	A

Figure 1 (continued 2)

ATOM	166	CB	LEU A	21	-13.417	-11.842	6.292	1.00	68.85	A
ATOM	167	CG	LEU A	21	-13.658	-11.701	7.797	1.00	69.20	A
ATOM	168	CD1	LEU A	21	-15.091	-11.257	8.058	1.00	69.44	A
ATOM	169	CD2	LEU A	21	-13.383	-13.037	8.473	1.00	69.17	A
ATOM	170	C	LEU A	21	-12.744	-9.468	5.837	1.00	69.92	A
ATOM	171	O	LEU A	21	-11.823	-9.033	5.133	1.00	70.14	A
ATOM	172	N	GLY A	22	-13.029	-8.981	7.043	1.00	70.90	A
ATOM	173	CA	GLY A	22	-12.270	-7.883	7.608	1.00	72.13	A
ATOM	174	C	GLY A	22	-13.141	-6.650	7.685	1.00	73.06	A
ATOM	175	O	GLY A	22	-13.445	-6.156	8.773	1.00	73.37	A
ATOM	176	N	GLY A	23	-13.556	-6.165	6.518	1.00	73.72	A
ATOM	177	CA	GLY A	23	-14.395	-4.982	6.447	1.00	74.24	A
ATOM	178	C	GLY A	23	-15.796	-5.167	7.006	1.00	74.63	A
ATOM	179	O	GLY A	23	-16.645	-5.826	6.394	1.00	74.77	A
ATOM	180	N	ARG A	24	-16.028	-4.573	8.176	1.00	74.56	A
ATOM	181	CA	ARG A	24	-17.315	-4.624	8.865	1.00	74.14	A
ATOM	182	CB	ARG A	24	-18.178	-3.428	8.440	1.00	75.43	A
ATOM	183	CG	ARG A	24	-19.494	-3.302	9.198	1.00	77.04	A
ATOM	184	CD	ARG A	24	-20.297	-2.119	8.683	1.00	78.78	A
ATOM	185	NE	ARG A	24	-21.576	-1.972	9.373	1.00	80.11	A
ATOM	186	CZ	ARG A	24	-22.483	-1.049	9.068	1.00	80.78	A
ATOM	187	NH1	ARG A	24	-22.251	-0.188	8.084	1.00	81.08	A
ATOM	188	NH2	ARG A	24	-23.623	-0.988	9.744	1.00	81.03	A
ATOM	189	C	ARG A	24	-18.102	-5.919	8.655	1.00	72.74	A
ATOM	190	O	ARG A	24	-19.099	-5.940	7.932	1.00	73.15	A
ATOM	191	N	PRO A	25	-17.659	-7.021	9.280	1.00	71.00	A
ATOM	192	CD	PRO A	25	-16.401	-7.195	10.026	1.00	70.86	A
ATOM	193	CA	PRO A	25	-18.367	-8.297	9.129	1.00	69.14	A
ATOM	194	CB	PRO A	25	-17.526	-9.256	9.967	1.00	69.82	A
ATOM	195	CG	PRO A	25	-16.138	-8.670	9.855	1.00	70.46	A
ATOM	196	C	PRO A	25	-19.787	-8.152	9.673	1.00	67.21	A
ATOM	197	O	PRO A	25	-19.964	-7.852	10.852	1.00	67.34	A
ATOM	198	N	THR A	26	-20.794	-8.355	8.825	1.00	64.60	A
ATOM	199	CA	THR A	26	-22.184	-8.218	9.265	1.00	61.62	A
ATOM	200	CB	THR A	26	-23.179	-8.457	8.100	1.00	62.41	A
ATOM	201	OG1	THR A	26	-22.829	-7.625	6.986	1.00	62.97	A
ATOM	202	CG2	THR A	26	-24.598	-8.102	8.535	1.00	62.89	A
ATOM	203	C	THR A	26	-22.487	-9.199	10.399	1.00	58.62	A
ATOM	204	O	THR A	26	-21.891	-9.105	11.474	1.00	58.71	A
ATOM	205	N	LEU A	27	-23.413	-10.128	10.167	1.00	54.49	A
ATOM	206	CA	LEU A	27	-23.766	-11.123	11.177	1.00	49.96	A
ATOM	207	CB	LEU A	27	-24.522	-12.298	10.546	1.00	50.45	A
ATOM	208	CG	LEU A	27	-25.845	-12.037	9.828	1.00	50.99	A
ATOM	209	CD1	LEU A	27	-25.611	-11.122	8.637	1.00	51.87	A
ATOM	210	CD2	LEU A	27	-26.450	-13.356	9.361	1.00	51.62	A
ATOM	211	C	LEU A	27	-22.461	-11.627	11.791	1.00	46.57	A
ATOM	212	O	LEU A	27	-21.498	-11.909	11.076	1.00	45.78	A
ATOM	213	N	PRO A	28	-22.406	-11.734	13.125	1.00	42.86	A
ATOM	214	CD	PRO A	28	-23.458	-11.471	14.125	1.00	42.50	A
ATOM	215	CA	PRO A	28	-21.179	-12.207	13.770	1.00	39.77	A
ATOM	216	CB	PRO A	28	-21.586	-12.325	15.243	1.00	40.55	A
ATOM	217	CG	PRO A	28	-22.641	-11.263	15.384	1.00	41.64	A
ATOM	218	C	PRO A	28	-20.704	-13.536	13.197	1.00	36.67	A
ATOM	219	O	PRO A	28	-19.502	-13.737	12.978	1.00	35.24	A
ATOM	220	N	ILE A	29	-21.659	-14.434	12.964	1.00	33.25	A
ATOM	221	CA	ILE A	29	-21.389	-15.764	12.440	1.00	31.49	A
ATOM	222	CB	ILE A	29	-22.725	-16.518	12.190	1.00	32.34	A
ATOM	223	CG2	ILE A	29	-23.443	-15.893	11.009	1.00	32.60	A
ATOM	224	CG1	ILE A	29	-22.486	-18.006	11.925	1.00	33.89	A
ATOM	225	CD1	ILE A	29	-22.008	-18.774	13.115	1.00	33.09	A
ATOM	226	C	ILE A	29	-20.600	-15.694	11.137	1.00	29.03	A
ATOM	227	O	ILE A	29	-19.779	-16.569	10.860	1.00	27.06	A
ATOM	228	N	LEU A	30	-20.810	-14.645	10.352	1.00	27.42	A
ATOM	229	CA	LEU A	30	-20.124	-14.555	9.059	1.00	26.34	A
ATOM	230	CB	LEU A	30	-20.837	-13.539	8.153	1.00	27.73	A
ATOM	231	CG	LEU A	30	-22.319	-13.856	7.930	1.00	29.16	A
ATOM	232	CD1	LEU A	30	-22.901	-12.767	7.025	1.00	29.49	A
ATOM	233	CD2	LEU A	30	-22.528	-15.249	7.312	1.00	28.59	A
ATOM	234	C	LEU A	30	-18.640	-14.238	9.154	1.00	24.62	A
ATOM	235	O	LEU A	30	-17.910	-14.362	8.168	1.00	24.88	A
ATOM	236	N	GLY A	31	-18.190	-13.860	10.350	1.00	21.78	A
ATOM	237	CA	GLY A	31	-16.789	-13.553	10.548	1.00	21.58	A
ATOM	238	C	GLY A	31	-16.069	-14.788	11.093	1.00	19.65	A
ATOM	239	O	GLY A	31	-14.889	-14.720	11.414	1.00	21.22	A
ATOM	240	N	ASN A	32	-16.784	-15.895	11.182	1.00	19.33	A
ATOM	241	CA	ASN A	32	-16.221	-17.164	11.678	1.00	17.81	A
ATOM	242	CB	ASN A	32	-17.174	-17.859	12.668	1.00	18.05	A
ATOM	243	CG	ASN A	32	-17.079	-17.275	14.077	1.00	14.39	A
ATOM	244	OD1	ASN A	32	-16.566	-16.193	14.234	1.00	18.82	A
ATOM	245	ND2	ASN A	32	-17.541	-18.018	15.082	1.00	16.05	A
ATOM	246	C	ASN A	32	-16.006	-18.109	10.524	1.00	19.88	A
ATOM	247	O	ASN A	32	-16.554	-17.930	9.426	1.00	20.74	A
ATOM	248	N	LEU A	33	-15.178	-19.116	10.781	1.00	19.03	A
ATOM	249	CA	LEU A	33	-14.924	-20.155	9.804	1.00	18.58	A
ATOM	250	CB	LEU A	33	-13.435	-20.435	9.671	1.00	20.53	A
ATOM	251	CG	LEU A	33	-12.569	-19.411	8.996	1.00	22.72	A
ATOM	252	CD1	LEU A	33	-11.137	-19.964	8.958	1.00	25.09	A
ATOM	253	CD2	LEU A	33	-13.107	-19.134	7.606	1.00	25.02	A
ATOM	254	C	LEU A	33	-15.530	-21.398	10.365	1.00	18.12	A
ATOM	255	O	LEU A	33	-15.430	-21.648	11.576	1.00	17.01	A
ATOM	256	N	LEU A	34	-16.184	-22.179	9.513	1.00	15.99	A
ATOM	257	CA	LEU A	34	-16.730	-23.433	9.951	1.00	16.00	A
ATOM	258	CB	LEU A	34	-17.914	-23.864	9.073	1.00	18.73	A
ATOM	259	CG	LEU A	34	-18.416	-25.301	9.197	1.00	17.56	A
ATOM	260	CD1	LEU A	34	-18.968	-25.610	10.583	1.00	20.61	A
ATOM	261	CD2	LEU A	34	-19.527	-25.480	8.138	1.00	20.63	A
ATOM	262	C	LEU A	34	-15.618	-24.467	9.807	1.00	17.87	A
ATOM	263	O	LEU A	34	-15.009	-24.561	8.725	1.00	18.24	A
ATOM	264	N	LEU A	35	-15.335	-25.196	10.893	1.00	16.38	A
ATOM	265	CA	LEU A	35	-14.346	-26.290	10.903	1.00	16.62	A

Figure 1 (continued 3)

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ATOM    266   CB    LEU A   35     -13.301  -26.110   12.029   1.00  16.55        A
ATOM    267   CG    LEU A   35     -12.328  -24.919   11.927   1.00  20.44        A
ATOM    268   CD1   LEU A   35     -13.026  -23.564   11.887   1.00  26.52        A
ATOM    269   CD2   LEU A   35     -11.438  -24.958   13.149   1.00  22.52        A
ATOM    270   C     LEU A   35     -15.083  -27.609   11.117   1.00  16.64        A
ATOM    271   O     LEU A   35     -15.859  -27.763   12.066   1.00  15.83        A
ATOM    272   N     GLN A   36     -14.857  -28.572   10.227   1.00  15.28        A
ATOM    273   CA    GLN A   36     -15.520  -29.866   10.344   1.00  15.61        A
ATOM    274   CB    GLN A   36     -16.596  -29.997    9.238   1.00  17.87        A
ATOM    275   CG    GLN A   36     -17.676  -28.913    9.217   1.00  23.26        A
ATOM    276   CD    GLN A   36     -18.504  -28.948    7.921   1.00  27.12        A
ATOM    277   OE1   GLN A   36     -19.714  -29.221    7.953   1.00  31.11        A
ATOM    278   NE2   GLN A   36     -17.850  -28.676    6.775   1.00  26.03        A
ATOM    279   C     GLN A   36     -14.507  -30.996   10.156   1.00  16.00        A
ATOM    280   O     GLN A   36     -13.767  -30.971    9.177   1.00  17.23        A
ATOM    281   N     VAL A   37     -14.461  -31.947   11.097   1.00  14.69.       A
ATOM    282   CA    VAL A   37     -13.594  -33.123   10.959   1.00  15.63        A
ATOM    283   CB    VAL A   37     -12.796  -33.403   12.236   1.00  14.73        A
ATOM    284   CG1   VAL A   37     -12.146  -34.774   12.143   1.00  16.16        A
ATOM    285   CG2   VAL A   37     -11.774  -32.274   12.445   1.00  14.31        A
ATOM    286   C     VAL A   37     -14.508  -34.322   10.684   1.00  17.15        A
ATOM    287   O     VAL A   37     -15.380  -34.665   11.495   1.00  16.68        A
ATOM    288   N     ALA A   38     -14.325  -34.947    9.525   1.00  18.78        A
ATOM    289   CA    ALA A   38     -15.146  -36.114    9.157   1.00  19.67        A
ATOM    290   CB    ALA A   38     -16.354  -35.671    8.393   1.00  19.20        A
ATOM    291   C     ALA A   38     -14.273  -36.995    8.288   1.00  21.68        A
ATOM    292   O     ALA A   38     -13.526  -36.475    7.460   1.00  20.43        A
ATOM    293   N     ASP A   39     -14.380  -38.312    8.476   1.00  23.51        A
ATOM    294   CA    ASP A   39     -13.554  -39.266    7.746   1.00  27.39        A
ATOM    295   CB    ASP A   39     -13.801  -39.139    6.244   1.00  30.92        A
ATOM    296   CG    ASP A   39     -13.805  -40.490    5.533   1.00  35.17        A
ATOM    297   OD1   ASP A   39     -13.575  -41.528    6.196   1.00  37.93        A
ATOM    298   OD2   ASP A   39     -14.044  -40.515    4.303   1.00  38.02        A
ATOM    299   C     ASP A   39     -12.136  -38.837    8.140   1.00  26.49        A
ATOM    300   O     ASP A   39     -11.870  -38.606    9.310   1.00  29.24        A
ATOM    301   N     GLY A   40     -11.226  -38.693    7.199   1.00  26.55        A
ATOM    302   CA    GLY A   40      -9.893  -38.278    7.614   1.00  22.82        A
ATOM    303   C     GLY A   40      -9.611  -36.884    7.084   1.00  20.99        A
ATOM    304   O     GLY A   40      -8.488  -36.548    6.730   1.00  20.13        A
ATOM    305   N     THR A   41     -10.640  -36.059    7.061   1.00  17.70        A.
ATOM    306   CA    THR A   41     -10.528  -34.735    6.493   1.00  17.27        A
ATOM    307   CB    THR A   41     -11.407  -34.671    5.199   1.00  19.00        A
ATOM    308   OG1   THR A   41     -11.050  -35.775    4.341   1.00  23.54        A
ATOM    309   CG2   THR A   41     -11.215  -33.363    4.457   1.00  22.95        A
ATOM    310   C     THR A   41     -10.974  -33.587    7.389   1.00  16.76        A
ATOM    311   O     THR A   41     -11.921  -33.718    8.136   1.00  18.19        A
ATOM    312   N     LEU A   42     -10.251  -32.483    7.332   1.00  14.51        A
ATOM    313   CA    LEU A   42     -10.668  -31.272    8.035   1.00  13.60        A
ATOM    314   CB    LEU A   42      -9.461  -30.576    8.698   1.00  14.21        A
ATOM    315   CG    LEU A   42      -9.719  -29.130    9.112   1.00  12.61        A
ATOM    316   CD1   LEU A   42     -10.808  -29.020   10.222   1.00  13.95        A
ATOM    317   CD2   LEU A   42      -8.374  -28.566    9.579   1.00  15.96        A
ATOM    318   C     LEU A   42     -11.170  -30.377    6.914   1.00  15.92        A
ATOM    319   O     LEU A   42     -10.443  -30.104    5.951   1.00  15.29        A
ATOM    320   N     SER A   43     -12.413  -29.907    7.016   1.00  13.67        A
ATOM    321   CA    SER A   43     -12.914  -28.978    6.009   1.00  14.02        A
ATOM    322   CB    SER A   43     -14.287  -29.408    5.481   1.00  15.11        A
ATOM    323   OG    SER A   43     -14.202  -30.670    4.815   1.00  15.94        A.
ATOM    324   C     SER A   43     -13.020  -27.623    6.675   1.00  14.81        A
ATOM    325   O     SER A   43     -13.360  -27.526    7.866   1.00  14.63        A
ATOM    326   N     LEU A   44     -12.706  -26.571    5.928   1.00  13.45        A
ATOM    327   CA    LEU A   44     -12.770  -25.220    6.475   1.00  13.96        A
ATOM    328   CB    LEU A   44     -11.379  -24.576    6.501   1.00  16.23        A
ATOM    329   CG    LEU A   44     -10.224  -25.221    7.264   1.00  19.59        A
ATOM    330   CD1   LEU A   44     -10.661  -25.513    8.708   1.00  23.82        A
ATOM    331   CD2   LEU A   44      -9.736  -26.446    6.550   1.00  22.21        A
ATOM    332   C     LEU A   44     -13.643  -24.408    5.547   1.00  17.42        A
ATOM    333   O     LEU A   44     -13.411  -24.421    4.336   1.00  17.59        A
ATOM    334   N     THR A   45     -14.624  -23.682    6.087   1.00  15.58        A
ATOM    335   CA    THR A   45     -15.517  -22.913    5.221   1.00  18.70        A
ATOM    336   CB    THR A   45     -16.922  -23.570    5.153   1.00  18.52        A
ATOM    337   OG1   THR A   45     -16.816  -24.941    4.706   1.00  18.50        A
ATOM    338   CG2   THR A   45     -17.837  -22.792    4.165   1.00  18.61        A
ATOM    339   C     THR A   45     -15.702  -21.465    5.653   1.00  19.93        A
ATOM    340   O     THR A   45     -15.915  -21.185    6.844   1.00  20.27        A
ATOM    341   N     GLY A   46     -15.617  -20.555    4.687   1.00  18.64        A
ATOM    342   CA    GLY A   46     -15.837  -19.129    4.940   1.00  20.18        A
ATOM    343   C     GLY A   46     -17.022  -18.682    4.090   1.00  20.92        A
ATOM    344   O     GLY A   46     -17.233  -19.247    3.011   1.00  20.00        A
ATOM    345   N     THR A   47     -17.816  -17.692    4.537   1.00  20.46        A
ATOM    346   CA    THR A   47     -18.967  -17.267    3.729   1.00  22.40        A
ATOM    347   CB    THR A   47     -20.188  -18.213    3.916   1.00  23.17        A
ATOM    348   OG1   THR A   47     -21.242  -17.858    2.999   1.00  23.27        A
ATOM    349   CG2   THR A   47     -20.745  -18.108    5.349   1.00  25.43        A
ATOM    350   C     THR A   47     -19.440  -15.864    4.085   1.00  23.69        A
ATOM    351   O     THR A   47     -19.201  -15.400    5.200   1.00  24.49        A
ATOM    352   N     ASP A   48     -20.108  -15.199    3.149   1.00  23.27        A
ATOM    353   CA    ASP A   48     -20.664  -13.857    3.407   1.00  22.37        A
ATOM    354   CB    ASP A   48     -19.905  -12.780    2.621   1.00  24.34        A
ATOM    355   CG    ASP A   48     -20.123  -12.864    1.121   1.00  24.11        A
ATOM    356   OD1   ASP A   48     -20.826  -13.780    0.658   1.00  22.62        A
ATOM    357   OD2   ASP A   48     -19.586  -12.001    0.407   1.00  28.57        A
ATOM    358   C     ASP A   48     -22.155  -13.856    3.053   1.00  23.86        A
ATOM    359   O     ASP A   48     -22.800  -12.787    2.957   1.00  22.46        A
ATOM    360   N     LEU A   49     -22.690  -15.069    2.911   1.00  21.60        A
ATOM    361   CA    LEU A   49     -24.084  -15.347    2.568   1.00  23.11        A
ATOM    362   CB    LEU A   49     -25.043  -14.351    3.236   1.00  24.46        A
ATOM    363   CG    LEU A   49     -25.225  -14.479    4.744   1.00  26.70        A
ATOM    364   CD1   LEU A   49     -26.124  -13.337    5.190   1.00  27.13        A
ATOM    365   CD2   LEU A   49     -25.795  -15.847    5.105   1.00  26.87        A
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Figure 1 (continued 4)

ATOM	366	C	LEU	A	49	-24.325	-15.305	1.067	1.00 20.63	A
ATOM	367	O	LEU	A	49	-25.268	-15.928	0.566	1.00 24.28	A
ATOM	368	N	GLU	A	50	-23.484	-14.575	0.346	1.00 19.18	A
ATOM	369	CA	GLU	A	50	-23.652	-14.494	-1.097	1.00 19.11	A
ATOM	370	CB	GLU	A	50	-23.243	-13.110	-1.610	1.00 21.43	A
ATOM	371	CG	GLU	A	50	-23.515	-12.896	-3.113	1.00 27.31	A
ATOM	372	CD	GLU	A	50	-23.235	-11.458	-3.604	1.00 28.85	A
ATOM	373	OE1	GLU	A	50	-22.085	-10.968	-3.454	1.00 31.33	A
ATOM	374	OE2	GLU	A	50	-24.168	-10.822	-4.172	1.00 31.83	A
ATOM	375	C	GLU	A	50	-22.787	-15.559	-1.758	1.00 20.12	A
ATOM	376	O	GLU	A	50	-23.166	-16.124	-2.786	1.00 19.05	A
ATOM	377	N	MET	A	51	-21.651	-15.846	-1.127	1.00 18.26	A
ATOM	378	CA	MET	A	51	-20.698	-16.832	-1.670	1.00 18.26	A
ATOM	379	CB	MET	A	51	-19.643	-16.116	-2.504	1.00 19.67	A
ATOM	380	CG	MET	A	51	-18.947	-15.032	-1.780	1.00 22.10	A
ATOM	381	SD	MET	A	51	-18.086	-14.041	-2.993	1.00 25.87	A
ATOM	382	CE	MET	A	51	-16.514	-14.275	-2.397	1.00 27.36	A
ATOM	383	C	MET	A	51	-20.053	-17.576	-0.525	1.00 18.84	A
ATOM	384	O	MET	A	51	-20.102	-17.129	0.634	1.00 18.64	A
ATOM	385	N	GLU	A	52	-19.428	-18.699	-0.853	1.00 16.68	A
ATOM	386	CA	GLU	A	52	-18.839	-19.572	0.152	1.00 19.13	A
ATOM	387	CB	GLU	A	52	-19.901	-20.637	0.452	1.00 22.65	A
ATOM	388	CG	GLU	A	52	-19.554	-21.806	1.323	1.00 32.13	A
ATOM	389	CD	GLU	A	52	-20.803	-22.623	1.650	1.00 34.31	A
ATOM	390	OE1	GLU	A	52	-20.682	-23.671	2.325	1.00 38.54	A
ATOM	391	OE2	GLU	A	52	-21.913	-22.211	1.235	1.00 36.05	A
ATOM	392	C	GLU	A	52	-17.595	-20.188	-0.449	1.00 18.25	A
ATOM	393	O	GLU	A	52	-17.555	-20.488	-1.639	1.00 17.91	A
ATOM	394	N	MET	A	53	-16.584	-20.356	0.377	1.00 18.60	A
ATOM	395	CA	MET	A	53	-15.339	-20.955	-0.074	1.00 17.33	A
ATOM	396	CB	MET	A	53	-14.202	-19.930	-0.036	1.00 21.43	A
ATOM	397	CG	MET	A	53	-12.851	-20.502	-0.484	1.00 26.15	A
ATOM	398	SD	MET	A	53	-12.771	-20.914	-2.256	1.00 32.73	A
ATOM	399	CE	MET	A	53	-12.410	-19.257	-2.959	1.00 30.62	A
ATOM	400	C	MET	A	53	-15.051	-22.112	0.886	1.00 17.68	A
ATOM	401	O	MET	A	53	-15.069	-21.933	2.102	1.00 17.40	A
ATOM	402	N	VAL	A	54	-14.786	-23.294	0.338	1.00 15.12	A
ATOM	403	CA	VAL	A	54	-14.507	-24.468	1.162	1.00 16.82	A
ATOM	404	CB	VAL	A	54	-15.508	-25.612	0.914	1.00 17.64	A
ATOM	405	CG1	VAL	A	54	-15.224	-26.754	1.871	1.00 18.47	A
ATOM	406	CG2	VAL	A	54	-16.959	-25.117	1.098	1.00 21.00	A
ATOM	407	C	VAL	A	54	-13.139	-25.036	0.823	1.00 17.33	A
ATOM	408	O	VAL	A	54	-12.814	-25.201	-0.343	1.00 19.27	A
ATOM	409	N	ALA	A	55	-12.349	-25.363	1.848	1.00 15.10	A
ATOM	410	CA	ALA	A	55	-11.031	-25.973	1.611	1.00 13.30	A
ATOM	411	CB	ALA	A	55	-9.923	-25.043	2.056	1.00 15.71	A
ATOM	412	C	ALA	A	55	-10.929	-27.286	2.394	1.00 16.85	A
ATOM	413	O	ALA	A	55	-11.528	-27.433	3.451	1.00 16.80	A
ATOM	414	N	ARG	A	56	-10.138	-28.233	1.895	1.00 15.48	A
ATOM	415	CA	ARG	A	56	-9.989	-29.505	2.613	1.00 15.80	A
ATOM	416	CB	ARG	A	56	-10.566	-30.677	1.789	1.00 20.20	A
ATOM	417	CG	ARG	A	56	-12.018	-30.440	1.349	1.00 23.44	A
ATOM	418	CD	ARG	A	56	-12.819	-31.720	1.096	1.00 28.95	A
ATOM	419	NE	ARG	A	56	-14.035	-31.591	1.909	1.00 31.67	A
ATOM	420	CZ	ARG	A	56	-15.058	-30.787	1.625	1.00 32.95	A
ATOM	421	NH1	ARG	A	56	-15.053	-30.038	0.508	1.00 32.56	A
ATOM	422	NH2	ARG	A	56	-16.048	-30.668	2.503	1.00 29.00	A
ATOM	423	C	ARG	A	56	-8.515	-29.772	2.931	1.00 15.06	A
ATOM	424	O	ARG	A	56	-7.623	-29.430	2.131	1.00 16.17	A
ATOM	425	N	VAL	A	57	-8.273	-30.364	4.104	1.00 14.32	A
ATOM	426	CA	VAL	A	57	-6.919	-30.693	4.567	1.00 12.85	A
ATOM	427	CB	VAL	A	57	-6.481	-29.759	5.755	1.00 15.84	A
ATOM	428	CG1	VAL	A	57	-5.134	-30.198	6.297	1.00 17.83	A
ATOM	429	CG2	VAL	A	57	-6.452	-28.283	5.289	1.00 18.06	A
ATOM	430	C	VAL	A	57	-6.966	-32.141	5.049	1.00 13.46	A
ATOM	431	O	VAL	A	57	-7.853	-32.534	5.813	1.00 13.57	A
ATOM	432	N	ALA	A	58	-6.028	-32.968	4.596	1.00 12.91	A
ATOM	433	CA	ALA	A	58	-6.027	-34.351	5.050	1.00 13.63	A
ATOM	434	CB	ALA	A	58	-5.228	-35.213	4.062	1.00 16.31	A
ATOM	435	C	ALA	A	58	-5.423	-34.471	6.459	1.00 13.61	A
ATOM	436	O	ALA	A	58	-4.481	-33.740	6.807	1.00 15.06	A
ATOM	437	N	LEU	A	59	-5.997	-35.362	7.269	1.00 15.23	A
ATOM	438	CA	LEU	A	59	-5.558	-35.589	8.648	1.00 16.38	A
ATOM	439	CB	LEU	A	59	-6.748	-35.439	9.599	1.00 15.55	A
ATOM	440	CG	LEU	A	59	-7.384	-34.042	9.562	1.00 14.50	A
ATOM	441	CD1	LEU	A	59	-8.607	-34.021	10.509	1.00 15.98	A
ATOM	442	CD2	LEU	A	59	-6.364	-32.973	9.991	1.00 14.17	A
ATOM	443	C	LEU	A	59	-4.980	-36.986	8.804	1.00 20.00	A
ATOM	444	O	LEU	A	59	-5.702	-37.982	8.671	1.00 23.51	A
ATOM	445	N	VAL	A	60	-3.700	-37.070	9.138	1.00 20.91	A
ATOM	446	CA	VAL	A	60	-3.081	-38.379	9.305	1.00 22.99	A
ATOM	447	CB	VAL	A	60	-1.720	-38.472	8.532	1.00 21.30	A
ATOM	448	CG1	VAL	A	60	-0.726	-37.522	9.135	1.00 21.15	A
ATOM	449	CG2	VAL	A	60	-1.177	-39.910	8.545	1.00 24.79	A
ATOM	450	C	VAL	A	60	-2.861	-38.661	10.779	1.00 25.44	A
ATOM	451	O	VAL	A	60	-2.801	-39.830	11.197	1.00 26.02	A
ATOM	452	N	GLN	A	61	-2.761	-37.596	11.578	1.00 26.01	A
ATOM	453	CA	GLN	A	61	-2.551	-37.734	13.014	1.00 26.21	A
ATOM	454	CB	GLN	A	61	-1.962	-36.437	13.569	1.00 26.62	A
ATOM	455	CG	GLN	A	61	-0.643	-36.050	12.877	1.00 27.36	A
ATOM	456	CD	GLN	A	61	0.082	-34.866	13.534	1.00 29.51	A
ATOM	457	OE1	GLN	A	61	0.274	-34.851	14.750	1.00 30.47	A
ATOM	458	NE2	GLN	A	61	0.498	-33.881	12.726	1.00 28.34	A
ATOM	459	C	GLN	A	61	-3.893	-38.063	13.663	1.00 26.03	A
ATOM	460	O	GLN	A	61	-4.944	-37.822	13.065	1.00 26.37	A
ATOM	461	N	PRO	A	62	-3.878	-38.637	14.883	1.00 26.72	A
ATOM	462	CD	PRO	A	62	-2.749	-39.028	15.752	1.00 26.01	A
ATOM	463	CA	PRO	A	62	-5.159	-38.969	15.514	1.00 24.46	A
ATOM	464	CB	PRO	A	62	-4.758	-39.400	16.929	1.00 26.77	A
ATOM	465	CG	PRO	A	62	-3.406	-40.043	16.689	1.00 25.60	A

Figure 1 (continued 5)

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ATOM    466  C    PRO A  62      -6.098 -37.789  15.500  1.00 21.59           A
ATOM    467  O    PRO A  62      -5.693 -36.637  15.713  1.00 20.88           A
ATOM    468  N    HIS A  63      -7.361 -38.082  15.234  1.00 21.18           A
ATOM    469  CA   HIS A  63      -8.371 -37.046  15.179  1.00 17.84           A
ATOM    470  CB   HIS A  63      -8.475 -36.482  13.754  1.00 18.27           A
ATOM    471  CG   HIS A  63      -8.667 -37.536  12.708  1.00 18.43           A
ATOM    472  CD2  HIS A  63      -9.792 -38.061  12.170  1.00 20.08           A
ATOM    473  ND1  HIS A  63      -7.615 -38.203  12.120  1.00 20.69           A
ATOM    474  CE1  HIS A  63      -8.083 -39.097  11.260  1.00 21.51           A
ATOM    475  NE2  HIS A  63      -9.403 -39.030  11.272  1.00 22.48           A
ATOM    476  C    HIS A  63      -9.728 -37.601  15.597  1.00 18.21           A
ATOM    477  O    HIS A  63      -9.933 -38.834  15.643  1.00 20.01           A
ATOM    478  N    GLU A  64     -10.643 -36.686  15.907  1.00 16.87           A
ATOM    479  CA   GLU A  64     -11.993 -37.073  16.308  1.00 19.00           A
ATOM    480  CB   GLU A  64     -12.160 -36.905  17.813  1.00 20.97           A
ATOM    481  CG   GLU A  64     -11.224 -37.788  18.610  1.00 24.05           A
ATOM    482  CD   GLU A  64     -11.335 -37.528  20.090  1.00 29.25           A
ATOM    483  OE1  GLU A  64     -12.050 -36.577  20.463  1.00 30.33           A
ATOM    484  OE2  GLU A  64     -10.710 -38.277  20.873  1.00 32.20           A
ATOM    485  C    GLU A  64     -12.964 -36.181  15.567  1.00 17.16           A
ATOM    486  O    GLU A  64     -12.753 -34.976  15.435  1.00 18.02           A
ATOM    487  N    PRO A  65     -14.070 -36.758  15.084  1.00 17.24           A
ATOM    488  CD   PRO A  65     -14.424 -38.180  15.166  1.00 17.26           A
ATOM    489  CA   PRO A  65     -15.063 -35.988  14.344  1.00 16.23           A
ATOM    490  CB   PRO A  65     -15.982 -37.063  13.753  1.00 16.65           A
ATOM    491  CG   PRO A  65     -15.903 -38.171  14.775  1.00 17.89           A
ATOM    492  C    PRO A  65     -15.825 -34.969  15.143  1.00 16.81           A
ATOM    493  O    PRO A  65     -15.998 -35.076  16.372  1.00 18.43           A
ATOM    494  N    GLY A  66     -16.279 -33.965  14.415  1.00 16.40           A
ATOM    495  CA   GLY A  66     -17.048 -32.905  15.003  1.00 16.58           A
ATOM    496  C    GLY A  66     -16.925 -31.636  14.205  1.00 17.44           A
ATOM    497  O    GLY A  66     -16.181 -31.543  13.219  1.00 18.08           A
ATOM    498  N    ALA A  67     -17.655 -30.628  14.646  1.00 15.76           A
ATOM    499  CA   ALA A  67     -17.660 -29.360  13.958  1.00 16.07           A
ATOM    500  CB   ALA A  67     -18.734 -29.361  12.850  1.00 15.82           A
ATOM    501  C    ALA A  67     -17.946 -28.232  14.919  1.00 17.46           A
ATOM    502  O    ALA A  67     -18.623 -28.416  15.950  1.00 19.40           A
ATOM    503  N    THR A  68     -17.433 -27.070  14.570  1.00 16.43           A
ATOM    504  CA   THR A  68     -17.658 -25.853  15.337  1.00 16.34           A
ATOM    505  CB   THR A  68     -16.788 -25.805  16.626  1.00 16.66           A
ATOM    506  OG1  THR A  68     -17.221 -24.683  17.412  1.00 17.85           A
ATOM    507  CG2  THR A  68     -15.312 -25.634  16.291  1.00 16.50           A
ATOM    508  C    THR A  68     -17.290 -24.675  14.449  1.00 17.50           A
ATOM    509  O    THR A  68     -16.857 -24.867  13.309  1.00 18.15           A
ATOM    510  N    THR A  69     -17.492 -23.453  14.916  1.00 16.80           A
ATOM    511  CA   THR A  69     -17.069 -22.299  14.121  1.00 16.22           A
ATOM    512  CB   THR A  69     -18.267 -21.521  13.510  1.00 19.21           A
ATOM    513  OG1  THR A  69     -18.868 -20.676  14.500  1.00 19.12           A
ATOM    514  CG2  THR A  69     -19.314 -22.481  12.964  1.00 19.28           A
ATOM    515  C    THR A  69     -16.254 -21.394  15.053  1.00 17.37           A
ATOM    516  O    THR A  69     -16.542 -21.318  16.250  1.00 19.10           A
ATOM    517  N    VAL A  70     -15.228 -20.743  14.523  1.00 16.92           A
ATOM    518  CA   VAL A  70     -14.348 -19.854  15.311  1.00 16.96           A
ATOM    519  CB   VAL A  70     -12.994 -20.555  15.682  1.00 18.01           A
ATOM    520  CG1  VAL A  70     -13.223 -21.742  16.630  1.00 20.79           A
ATOM    521  CG2  VAL A  70     -12.305 -21.010  14.414  1.00 18.76           A
ATOM    522  C    VAL A  70     -14.000 -18.592  14.528  1.00 17.58           A
ATOM    523  O    VAL A  70     -14.107 -18.570  13.284  1.00 16.41           A
ATOM    524  N    PRO A  71     -13.576 -17.519  15.220  1.00 16.78           A
ATOM    525  CD   PRO A  71     -13.582 -17.315  16.689  1.00 17.77           A
ATOM    526  CA   PRO A  71     -13.224 -16.275  14.523  1.00 17.44           A
ATOM    527  CB   PRO A  71     -12.701 -15.398  15.633  1.00 19.39           A
ATOM    528  CG   PRO A  71     -13.616 -15.810  16.788  1.00 20.22           A
ATOM    529  C    PRO A  71     -12.184 -16.546  13.451  1.00 17.20           A
ATOM    530  O    PRO A  71     -11.091 -16.993  13.744  1.00 17.02           A
ATOM    531  N    ALA A  72     -12.522 -16.251  12.204  1.00 16.42           A
ATOM    532  CA   ALA A  72     -11.610 -16.566  11.126  1.00 16.85           A
ATOM    533  CB   ALA A  72     -12.325 -16.376   9.776  1.00 18.54           A
ATOM    534  C    ALA A  72     -10.294 -15.813  11.128  1.00 17.52           A
ATOM    535  O    ALA A  72      -9.225 -16.433  10.975  1.00 17.07           A
ATOM    536  N    ARG A  73     -10.342 -14.492  11.276  1.00 16.94           A
ATOM    537  CA   ARG A  73      -9.109 -13.711  11.242  1.00 19.22           A
ATOM    538  CB   ARG A  73      -9.394 -12.209  11.247  1.00 23.69           A
ATOM    539  CG   ARG A  73      -8.138 -11.345  10.965  1.00 28.94           A
ATOM    540  CD   ARG A  73      -7.648 -11.495   9.517  1.00 34.56           A
ATOM    541  NE   ARG A  73      -6.218 -11.192   9.385  1.00 39.05           A
ATOM    542  CZ   ARG A  73      -5.513 -11.337   8.262  1.00 40.82           A
ATOM    543  NH1  ARG A  73      -6.102 -11.781   7.155  1.00 42.67           A
ATOM    544  NH2  ARG A  73      -4.217 -11.044   8.246  1.00 41.48           A
ATOM    545  C    ARG A  73      -8.202 -14.053  12.420  1.00 18.20           A
ATOM    546  O    ARG A  73      -6.988 -14.203  12.260  1.00 17.86           A
ATOM    547  N    LYS A  74      -8.794 -14.201  13.595  1.00 17.94           A
ATOM    548  CA   LYS A  74      -7.998 -14.536  14.762  1.00 17.40           A
ATOM    549  CB   LYS A  74      -8.853 -14.517  16.023  1.00 17.77           A
ATOM    550  CG   LYS A  74      -9.201 -13.129  16.534  1.00 19.95           A
ATOM    551  CD   LYS A  74     -10.300 -13.274  17.579  1.00 20.83           A
ATOM    552  CE   LYS A  74     -10.701 -11.937  18.146  1.00 21.69           A
ATOM    553  NZ   LYS A  74     -11.934 -12.085  18.959  1.00 18.53           A
ATOM    554  C    LYS A  74      -7.364 -15.910  14.608  1.00 15.84           A
ATOM    555  O    LYS A  74      -6.181 -16.077  14.902  1.00 16.97           A
ATOM    556  N    PHE A  75      -8.128 -16.896  14.144  1.00 16.01           A
ATOM    557  CA   PHE A  75      -7.565 -18.241  13.996  1.00 16.50           A
ATOM    558  CB   PHE A  75      -8.667 -19.271  13.657  1.00 15.00           A
ATOM    559  CG   PHE A  75      -8.176 -20.690  13.548  1.00 17.05           A
ATOM    560  CD1  PHE A  75      -7.463 -21.292  14.585  1.00 18.49           A
ATOM    561  CD2  PHE A  75      -8.449 -21.441  12.409  1.00 18.78           A
ATOM    562  CE1  PHE A  75      -7.031 -22.619  14.485  1.00 19.50           A
ATOM    563  CE2  PHE A  75      -8.011 -22.784  12.300  1.00 20.42           A
ATOM    564  CZ   PHE A  75      -7.303 -23.364  13.339  1.00 17.99           A
ATOM    565  C    PHE A  75      -6.451 -18.217  12.947  1.00 15.71           A
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Figure 1 (continued 6)

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ATOM    566  O    PHE A  75                -5.377 -18.772  13.158  1.00 15.69           A
ATOM    567  N    PHE A  76                -6.671 -17.524  11.821  1.00 15.86           A
ATOM    568  CA   PHE A  76                -5.625 -17.426  10.800  1.00 15.67           A
ATOM    569  CB   PHE A  76                -6.182 -16.680   9.572  1.00 16.48           A
ATOM    570  CG   PHE A  76                -5.186 -16.476   8.472  1.00 20.93           A
ATOM    571  CD1  PHE A  76                -4.368 -17.506   8.049  1.00 20.82           A
ATOM    572  CD2  PHE A  76                -5.108 -15.250   7.830  1.00 25.97           A
ATOM    573  CE1  PHE A  76                -3.481 -17.330   6.996  1.00 22.93           A
ATOM    574  CE2  PHE A  76                -4.219 -15.058   6.761  1.00 27.38           A
ATOM    575  CZ   PHE A  76                -3.407 -16.104   6.348  1.00 24.82           A
ATOM    576  C    PHE A  76                -4.366 -16.709  11.335  1.00 16.51           A
ATOM    577  O    PHE A  76                -3.244 -17.182  11.129  1.00 15.99           A
ATOM    578  N    ASP A  77                -4.544 -15.583  12.027  1.00 14.50           A
ATOM    579  CA   ASP A  77                -3.387 -14.859  12.560  1.00 17.13           A
ATOM    580  CB   ASP A  77                -3.832 -13.526  13.167  1.00 19.74           A
ATOM    581  CG   ASP A  77                -4.227 -12.510  12.107  1.00 23.30           A
ATOM    582  OD1  ASP A  77                -3.860 -12.698  10.926  1.00 23.00           A
ATOM    583  OD2  ASP A  77                -4.897 -11.515  12.465  1.00 24.82           A
ATOM    584  C    ASP A  77                -2.618 -15.695  13.590  1.00 16.29           A
ATOM    585  O    ASP A  77                -1.399 -15.629  13.647  1.00 16.00           A
ATOM    586  N    ILE A  78                -3.325 -16.465  14.414  1.00 15.43           A
ATOM    587  CA   ILE A  78                -2.633 -17.306  15.393  1.00 15.62           A
ATOM    588  CB   ILE A  78                -3.649 -18.030  16.297  1.00 16.32           A
ATOM    589  CG2  ILE A  78                -2.968 -19.174  17.072  1.00 17.56           A
ATOM    590  CG1  ILE A  78                -4.258 -17.015  17.275  1.00 17.00           A
ATOM    591  CD1  ILE A  78                -5.491 -17.573  18.024  1.00 17.64           A
ATOM    592  C    ILE A  78                -1.809 -18.354  14.652  1.00 16.31           A
ATOM    593  O    ILE A  78                -0.634 -18.563  14.949  1.00 16.75           A
ATOM    594  N    CYS A  79                -2.413 -19.013  13.676  1.00 14.73           A
ATOM    595  CA   CYS A  79                -1.665 -20.046  12.938  1.00 15.03           A
ATOM    596  CB   CYS A  79                -2.603 -20.761  11.979  1.00 16.89           A
ATOM    597  SG   CYS A  79                -3.823 -21.817  12.844  1.00 17.54           A
ATOM    598  C    CYS A  79                -0.456 -19.455  12.192  1.00 16.05           A
ATOM    599  O    CYS A  79                 0.649 -19.988  12.265  1.00 17.02           A
ATOM    600  N    ARG A  80                -0.669 -18.337  11.512  1.00 16.19           A
ATOM    601  CA   ARG A  80                 0.393 -17.690  10.775  1.00 16.85           A
ATOM    602  CB   ARG A  80                -0.188 -16.537   9.946  1.00 20.00           A
ATOM    603  CG   ARG A  80                 0.778 -15.991   8.885  1.00 27.92           A
ATOM    604  CD   ARG A  80                 0.031 -15.082   7.905  1.00 32.53           A
ATOM    605  NE   ARG A  80                -0.726 -14.049   8.612  1.00 35.79           A
ATOM    606  CZ   ARG A  80                -0.172 -13.067   9.323  1.00 37.31           A
ATOM    607  NH1  ARG A  80                 1.152 -12.973   9.420  1.00 38.32           A
ATOM    608  NH2  ARG A  80                -0.944 -12.190   9.956  1.00 37.64           A
ATOM    609  C    ARG A  80                 1.494 -17.166  11.704  1.00 15.48           A
ATOM    610  O    ARG A  80                 2.671 -17.183  11.330  1.00 16.18           A
ATOM    611  N    GLY A  81                 1.126 -16.734  12.920  1.00 13.81           A
ATOM    612  CA   GLY A  81                 2.092 -16.185  13.853  1.00 15.77           A
ATOM    613  C    GLY A  81                 2.971 -17.205  14.540  1.00 15.13           A
ATOM    614  O    GLY A  81                 3.993 -16.858  15.138  1.00 15.06           A
ATOM    615  N    LEU A  82                 2.558 -18.463  14.470  1.00 13.35           A
ATOM    616  CA   LEU A  82                 3.351 -19.550  15.059  1.00 13.35           A
ATOM    617  CB   LEU A  82                 2.525 -20.845  15.156  1.00 12.49           A
ATOM    618  CG   LEU A  82                 1.493 -20.791  16.304  1.00 12.47           A
ATOM    619  CD1  LEU A  82                 0.486 -21.910  16.176  1.00 12.91           A
ATOM    620  CD2  LEU A  82                 2.215 -20.852  17.693  1.00 14.10           A
ATOM    621  C    LEU A  82                 4.565 -19.749  14.158  1.00 15.03           A
ATOM    622  O    LEU A  82                 4.527 -19.404  12.963  1.00 15.46           A
ATOM    623  N    PRO A  83                 5.645 -20.316  14.709  1.00 16.44           A
ATOM    624  CD   PRO A  83                 5.747 -20.916  16.057  1.00 16.82           A
ATOM    625  CA   PRO A  83                 6.868 -20.532  13.940  1.00 17.96           A
ATOM    626  CB   PRO A  83                 7.878 -20.913  15.013  1.00 17.93           A
ATOM    627  CG   PRO A  83                 7.049 -21.726  15.978  1.00 17.83           A
ATOM    628  C    PRO A  83                 6.792 -21.560  12.827  1.00 19.15           A
ATOM    629  O    PRO A  83                 5.974 -22.483  12.842  1.00 16.64           A
ATOM    630  N    GLU A  84                 7.647 -21.362  11.834  1.00 18.77           A
ATOM    631  CA   GLU A  84                 7.720 -22.297  10.724  1.00 20.63           A
ATOM    632  CB   GLU A  84                 8.866 -21.879   9.798  1.00 23.64           A
ATOM    633  CG   GLU A  84                 9.092 -22.783   8.594  1.00 31.62           A
ATOM    634  CD   GLU A  84                10.336 -22.356   7.829  1.00 36.15           A
ATOM    635  OE1  GLU A  84                10.445 -21.139   7.504  1.00 39.83          ｜A
ATOM    636  OE2  GLU A  84                11.206 -23.221   7.567  1.00 40.03          ｜A
ATOM    637  C    GLU A  84                 7.978 -23.693  11.297  1.00 19.73           A
ATOM    638  O    GLU A  84                 8.801 -23.867  12.213  1.00 20.17           A
ATOM    639  N    GLY A  85                 7.262 -24.686  10.779  1.00 20.11           A
ATOM    640  CA   GLY A  85                 7.432 -26.046  11.263  1.00 19.52           A
ATOM    641  C    GLY A  85                 6.582 -26.430  12.465  1.00 19.27           A
ATOM    642  O    GLY A  85                 6.600 -27.576  12.919  1.00 21.77           A
ATOM    643  N    ALA A  86                 5.825 -25.479  12.996  1.00 16.80           A
ATOM    644  CA   ALA A  86                 4.989 -25.776  14.152  1.00 16.45           A
ATOM    645  CB   ALA A  86                 4.313 -24.490  14.661  1.00 16.16           A
ATOM    646  C    ALA A  86                 3.910 -26.805  13.839  1.00 16.34           A
ATOM    647  O    ALA A  86                 3.430 -26.884  12.703  1.00 16.48           A
ATOM    648  N    GLU A  87                 3.552 -27.584  14.857  1.00 15.82           A
ATOM    649  CA   GLU A  87                 2.479 -28.577  14.792  1.00 16.94           A
ATOM    650  CB   GLU A  87                 2.871 -29.867  15.511  1.00 20.12           A
ATOM    651  CG   GLU A  87                 3.869 -30.727  14.757  1.00 24.42           A
ATOM    652  CD   GLU A  87                 3.204 -31.527  13.643  1.00 29.00           A
ATOM    653  OE1  GLU A  87                 1.962 -31.445  13.512  1.00 30.19           A
ATOM    654  OE2  GLU A  87                 3.927 -32.242  12.902  1.00 33.75           A
ATOM    655  C    GLU A  87                 1.371 -27.889  15.598  1.00 16.68           A
ATOM    656  O    GLU A  87                 1.643 -27.315  16.669  1.00 16.47           A
ATOM    657  N    ILE A  88                 0.137 -27.956  15.112  1.00 15.63           A
ATOM    658  CA   ILE A  88                -0.964 -27.286  15.783  1.00 14.47           A
ATOM    659  CB   ILE A  88                -1.551 -26.225  14.815  1.00 14.61           A
ATOM    660  CG2  ILE A  88                -2.717 -25.471  15.455  1.00 15.66           A
ATOM    661  CG1  ILE A  88                -0.434 -25.252  14.413  1.00 16.03           A
ATOM    662  CD1  ILE A  88                -0.916 -24.176  13.495  1.00 15.45           A
ATOM    663  C    ILE A  88                -2.026 -28.285  16.215  1.00 13.85           A
ATOM    664  O    ILE A  88                -2.626 -28.982  15.376  1.00 14.57           A
ATOM    665  N    ALA A  89                -2.251 -28.360  17.529  1.00 12.25           A
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Figure 1 (continued 7)

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ATOM    666  CA   ALA A  89      -3.239  -29.289  18.093  1.00  12.02           A
ATOM    667  CB   ALA A  89      -2.659  -29.952  19.353  1.00  13.11           A
ATOM    668  C    ALA A  89      -4.472  -28.479  18.426  1.00  11.71           A
ATOM    669  O    ALA A  89      -4.399  -27.426  19.061  1.00  13.67           A
ATOM    670  N    VAL A  90      -5.626  -28.961  18.000  1.00  10.89           A
ATOM    671  CA   VAL A  90      -6.867  -28.214  18.186  1.00  12.44           A
ATOM    672  CB   VAL A  90      -7.383  -27.710  16.811  1.00  12.40           A
ATOM    673  CG1  VAL A  90      -8.769  -27.064  16.940  1.00  13.53           A
ATOM    674  CG2  VAL A  90      -6.412  -26.706  16.235  1.00  14.45           A
ATOM    675  C    VAL A  90      -7.922  -29.131  18.759  1.00  13.45           A
ATOM    676  O    VAL A  90      -8.095  -30.261  18.298  1.00  15.19           A
ATOM    677  N    GLN A  91      -8.636  -28.655  19.774  1.00  14.36           A
ATOM    678  CA   GLN A  91      -9.735  -29.465  20.314  1.00  14.06           A
ATOM    679  CB   GLN A  91      -9.285  -30.386  21.450  1.00  17.88           A
ATOM    680  CG   GLN A  91      -8.554  -29.714  22.519  1.00  21.85           A
ATOM    681  CD   GLN A  91      -7.719  -30.667  23.362  1.00  28.08           A
ATOM    682  OE1  GLN A  91      -7.236  -31.706  22.883  1.00  32.53           A
ATOM    683  NE2  GLN A  91      -7.514  -30.297  24.610  1.00  28.96           A
ATOM    684  C    GLN A  91     -10.861  -28.572  20.778  1.00  15.88           A
ATOM    685  O    GLN A  91     -10.662  -27.498  21.336  1.00  15.55           A
ATOM    686  N    LEU A  92     -12.076  -29.022  20.506  1.00  15.92           A
ATOM    687  CA   LEU A  92     -13.242  -28.290  20.937  1.00  18.46           A
ATOM    688  CB   LEU A  92     -14.426  -28.669  20.044  1.00  18.53           A
ATOM    689  CG   LEU A  92     -15.797  -28.084  20.379  1.00  19.11           A
ATOM    690  CD1  LEU A  92     -15.815  -26.567  20.190  1.00  17.67           A
ATOM    691  CD2  LEU A  92     -16.801  -28.748  19.451  1.00  19.82           A
ATOM    692  C    LEU A  92     -13.490  -28.723  22.370  1.00  19.94           A
ATOM    693  O    LEU A  92     -13.491  -29.938  22.675  1.00  20.27           A
ATOM    694  N    GLU A  93     -13.692  -27.737  23.242  1.00  21.27           A
ATOM    695  CA   GLU A  93     -13.950  -27.969  24.656  1.00  23.60           A
ATOM    696  CB   GLU A  93     -12.727  -27.593  25.472  1.00  24.28           A
ATOM    697  CG   GLU A  93     -11.502  -28.346  25.001  1.00  25.20           A
ATOM    698  CD   GLU A  93     -10.402  -28.368  26.037  1.00  26.28           A
ATOM    699  OE1  GLU A  93     -10.239  -27.343  26.732  1.00  28.86           A
ATOM    700  OE2  GLU A  93      -9.701  -29.405  26.152  1.00  26.10           A
ATOM    701  C    GLU A  93     -15.122  -27.105  25.061  1.00  24.07           A
ATOM    702  O    GLU A  93     -14.943  -26.031  25.640  1.00  25.47           A
ATOM    703  N    GLY A  94     -16.318  -27.570  24.726  1.00  26.68           A
ATOM    704  CA   GLY A  94     -17.517  -26.822  25.063  1.00  28.20           A
ATOM    705  C    GLY A  94     -17.675  -25.520  24.310  1.00  28.08           A
ATOM    706  O    GLY A  94     -17.807  -25.500  23.080  1.00  30.95           A
ATOM    707  N    GLU A  95     -17.668  -24.409  25.036  1.00  27.27           A
ATOM    708  CA   GLU A  95     -17.840  -23.109  24.405  1.00  26.17           A
ATOM    709  CB   GLU A  95     -18.429  -22.111  25.404  1.00  29.49           A
ATOM    710  CG   GLU A  95     -19.812  -22.514  25.947  1.00  34.68           A
ATOM    711  CD   GLU A  95     -20.819  -22.776  24.829  1.00  37.59           A
ATOM    712  OE1  GLU A  95     -20.860  -21.971  23.871  1.00  39.61           A
ATOM    713  OE2  GLU A  95     -21.568  -23.779  24.915  1.00  40.32           A
ATOM    714  C    GLU A  95     -16.561  -22.524  23.816  1.00  23.92           A
ATOM    715  O    GLU A  95     -16.603  -21.458  23.201  1.00  24.33           A
ATOM    716  N    ARG A  96     -15.429  -23.192  24.031  1.00  19.97           A
ATOM    717  CA   ARG A  96     -14.189  -22.685  23.489  1.00  18.11           A
ATOM    718  CB   ARG A  96     -13.242  -22.189  24.619  1.00  20.61           A
ATOM    719  CG   ARG A  96     -12.680  -23.267  25.616  1.00  22.85           A
ATOM    720  CD   ARG A  96     -11.343  -23.897  25.139  1.00  25.49           A
ATOM    721  NE   ARG A  96     -10.623  -24.711  26.143  1.00  24.91           A
ATOM    722  CZ   ARG A  96      -9.771  -24.241  27.058  1.00  25.23           A
ATOM    723  NH1  ARG A  96      -9.515  -22.942  27.120  1.00  26.05           A
ATOM    724  NH2  ARG A  96      -9.147  -25.086  27.903  1.00  20.77           A
ATOM    725  C    ARG A  96     -13.471  -23.726  22.666  1.00  15.35           A
ATOM    726  O    ARG A  96     -13.740  -24.924  22.790  1.00  15.87           A
ATOM    727  N    MET A  97     -12.609  -23.237  21.781  1.00  14.95           A
ATOM    728  CA   MET A  97     -11.789  -24.134  20.978  1.00  12.81           A
ATOM    729  CB   MET A  97     -11.921  -23.850  19.476  1.00  15.67           A
ATOM    730  CG   MET A  97     -11.205  -24.939  18.666  1.00  13.94           A
ATOM    731  SD   MET A  97     -11.365  -24.789  16.864  1.00  16.92           A
ATOM    732  CE   MET A  97      -9.931  -23.715  16.512  1.00  14.97           A
ATOM    733  C    MET A  97     -10.377  -23.860  21.444  1.00  12.28           A
ATOM    734  O    MET A  97      -9.912  -22.714  21.373  1.00  13.91           A
ATOM    735  N    LEU A  98      -9.697  -24.908  21.922  1.00  11.68           A
ATOM    736  CA   LEU A  98      -8.342  -24.751  22.424  1.00  11.70           A
ATOM    737  CB   LEU A  98      -8.137  -25.671  23.643  1.00  13.52           A
ATOM    738  CG   LEU A  98      -6.728  -25.651  24.249  1.00  15.75           A
ATOM    739  CD1  LEU A  98      -6.406  -24.288  24.856  1.00  16.82           A
ATOM    740  CD2  LEU A  98      -6.635  -26.764  25.314  1.00  17.18           A
ATOM    741  C    LEU A  98      -7.340  -25.091  21.327  1.00  11.06           A
ATOM    742  O    LEU A  98      -7.413  -26.162  20.715  1.00  13.52           A
ATOM    743  N    VAL A  99      -6.439  -24.155  21.081  1.00  11.82           A
ATOM    744  CA   VAL A  99      -5.357  -24.306  20.102  1.00  10.73           A
ATOM    745  CB   VAL A  99      -5.348  -23.106  19.112  1.00  10.91           A
ATOM    746  CG1  VAL A  99      -4.236  -23.307  18.079  1.00  13.86           A
ATOM    747  CG2  VAL A  99      -6.690  -23.022  18.393  1.00  13.77           A
ATOM    748  C    VAL A  99      -4.032  -24.330  20.855  1.00  11.36           A
ATOM    749  O    VAL A  99      -3.735  -23.418  21.637  1.00  12.82           A
ATOM    750  N    ARG A 100      -3.241  -25.378  20.621  1.00  11.29           A
ATOM    751  CA   ARG A 100      -1.951  -25.515  21.299  1.00  10.63           A
ATOM    752  CB   ARG A 100      -2.017  -26.687  22.287  1.00  12.67           A
ATOM    753  CG   ARG A 100      -3.028  -26.536  23.444  1.00  13.82           A
ATOM    754  CD   ARG A 100      -2.999  -27.792  24.309  1.00  18.46           A
ATOM    755  NE   ARG A 100      -3.557  -28.927  23.578  1.00  18.43           A
ATOM    756  CZ   ARG A 100      -2.969  -30.114  23.447  1.00  20.90           A
ATOM    757  NH1  ARG A 100      -1.779  -30.341  24.003  1.00  23.86           A
ATOM    758  NH2  ARG A 100      -3.571  -31.076  22.763  1.00  21.35           A
ATOM    759  C    ARG A 100      -0.818  -25.796  20.348  1.00  12.06           A
ATOM    760  O    ARG A 100      -0.952  -26.607  19.455  1.00  13.88           A
ATOM    761  N    SER A 101       0.319  -25.142  20.560  1.00  10.58           A
ATOM    762  CA   SER A 101       1.500  -25.414  19.734  1.00  12.72           A
ATOM    763  CB   SER A 101       1.457  -24.582  18.448  1.00  14.43           A
ATOM    764  OG   SER A 101       2.562  -24.907  17.600  1.00  14.52           A
ATOM    765  C    SER A 101       2.697  -25.036  20.597  1.00  13.21           A
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Figure 1 (continued 8)

ATOM	766	O	SER A 101	2.755	-23.917	21.070	1.00	12.38	A
ATOM	767	N	GLY A 102	3.655	-25.952	20.787	1.00	14.97	A
ATOM	768	CA	GLY A 102	4.787	-25.626	21.655	1.00	15.35	A
ATOM	769	C	GLY A 102	4.234	-25.239	23.022	1.00	14.72	A
ATOM	770	O	GLY A 102	3.396	-25.957	23.566	1.00	15.06	A
ATOM	771	N	ARG A 103	4.715	-24.127	23.580	1.00	14.39	A
ATOM	772	CA	ARG A 103	4.225	-23.632	24.861	1.00	15.53	A
ATOM	773	CB	ARG A 103	5.383	-23.301	25.800	1.00	16.98	A
ATOM	774	CG	ARG A 103	6.122	-24.596	26.170	1.00	18.28	A
ATOM	775	CD	ARG A 103	7.074	-24.407	27.335	1.00	22.26	A
ATOM	776	NE	ARG A 103	8.146	-23.480	27.027	1.00	24.02	A
ATOM	777	CZ	ARG A 103	9.048	-23.096	27.930	1.00	27.13	A
ATOM	778	NH1	ARG A 103	8.986	-23.567	29.177	1.00	28.33	A
ATOM	779	NH2	ARG A 103	10.000	-22.243	27.594	1.00	29.41	A
ATOM	780	C	ARG A 103	3.346	-22.402	24.617	1.00	15.01	A
ATOM	781	O	ARG A 103	3.318	-21.450	25.423	1.00	16.19	A
ATOM	782	N	SER A 104	2.650	-22.424	23.477	1.00	12.66	A
ATOM	783	CA	SER A 104	1.707	-21.349	23.143	1.00	11.12	A
ATOM	784	CB	SER A 104	1.917	-20.857	21.705	1.00	11.60	A
ATOM	785	OG	SER A 104	3.262	-20.458	21.462	1.00	11.97	A
ATOM	786	C	SER A 104	0.313	-21.971	23.254	1.00	13.02	A
ATOM	787	O	SER A 104	0.076	-23.082	22.774	1.00	13.52	A
ATOM	788	N	ARG A 105	-0.608	-21.251	23.895	1.00	11.22	A
ATOM	789	CA	ARG A 105	-1.991	-21.722	24.070	1.00	13.13	A
ATOM	790	CB	ARG A 105	-2.262	-22.132	25.534	1.00	14.88	A
ATOM	791	CG	ARG A 105	-1.481	-23.313	26.011	1.00	14.45	A
ATOM	792	CD	ARG A 105	-1.618	-23.515	27.546	1.00	14.09	A
ATOM	793	NE	ARG A 105	-3.010	-23.510	28.001	1.00	16.53	A
ATOM	794	CZ	ARG A 105	-3.784	-24.593	28.018	1.00	18.83	A
ATOM	795	NH1	ARG A 105	-3.293	-25.743	27.603	1.00	17.38	A
ATOM	796	NH2	ARG A 105	-5.054	-24.513	28.441	1.00	18.17	A
ATOM	797	C	ARG A 105	-2.956	-20.617	23.727	1.00	13.13	A
ATOM	798	O	ARG A 105	-2.750	-19.454	24.098	1.00	13.47	A
ATOM	799	N	PHE A 106	-4.036	-20.973	23.032	1.00	11.95	A
ATOM	800	CA	PHE A 106	-5.055	-19.984	22.687	1.00	12.74	A
ATOM	801	CB	PHE A 106	-4.909	-19.554	21.211	1.00	12.74	A
ATOM	802	CG	PHE A 106	-3.507	-19.127	20.851	1.00	13.12	A
ATOM	803	CD1	PHE A 106	-2.537	-20.086	20.549	1.00	13.32	A
ATOM	804	CD2	PHE A 106	-3.146	-17.791	20.918	1.00	13.88	A
ATOM	805	CE1	PHE A 106	-1.230	-19.724	20.331	1.00	13.59	A
ATOM	806	CE2	PHE A 106	-1.819	-17.406	20.702	1.00	15.45	A
ATOM	807	CZ	PHE A 106	-0.862	-18.385	20.411	1.00	13.62	A
ATOM	808	C	PHE A 106	-6.422	-20.606	22.881	1.00	12.43	A
ATOM	809	O	PHE A 106	-6.666	-21.731	22.464	1.00	13.63	A
ATOM	810	N	SER A 107	-7.322	-19.864	23.519	1.00	12.50	A
ATOM	811	CA	SER A 107	-8.683	-20.348	23.707	1.00	15.61	A
ATOM	812	CB	SER A 107	-9.056	-20.308	25.183	1.00	17.07	A
ATOM	813	OG	SER A 107	-10.401	-20.709	25.398	1.00	20.88	A
ATOM	814	C	SER A 107	-9.551	-19.357	22.940	1.00	14.70	A
ATOM	815	O	SER A 107	-9.596	-18.184	23.304	1.00	15.97	A
ATOM	816	N	LEU A 108	-10.219	-19.841	21.882	1.00	15.80	A
ATOM	817	CA	LEU A 108	-11.072	-19.012	21.039	1.00	15.44	A
ATOM	818	CB	LEU A 108	-10.829	-19.356	19.565	1.00	14.95	A
ATOM	819	CG	LEU A 108	-9.457	-18.953	19.034	1.00	15.14	A
ATOM	820	CD1	LEU A 108	-9.221	-19.543	17.631	1.00	17.32	A
ATOM	821	CD2	LEU A 108	-9.368	-17.437	19.028	1.00	18.64	A
ATOM	822	C	LEU A 108	-12.548	-19.248	21.305	1.00	14.24	A
ATOM	823	O	LEU A 108	-12.949	-20.357	21.612	1.00	14.91	A
ATOM	824	N	SER A 109	-13.347	-18.194	21.121	1.00	16.51	A
ATOM	825	CA	SER A 109	-14.789	-18.290	21.304	1.00	16.82	A
ATOM	826	CB	SER A 109	-15.426	-16.899	21.319	1.00	19.43	A
ATOM	827	OG	SER A 109	-15.108	-16.215	20.106	1.00	24.23	A
ATOM	828	C	SER A 109	-15.367	-19.064	20.138	1.00	17.73	A
ATOM	829	O	SER A 109	-14.799	-19.072	19.056	1.00	18.59	A
ATOM	830	N	THR A 110	-16.485	-19.728	20.364	1.00	16.33	A
ATOM	831	CA	THR A 110	-17.113	-20.485	19.277	1.00	17.92	A
ATOM	832	CB	THR A 110	-17.101	-22.013	19.518	1.00	18.59	A
ATOM	833	OG1	THR A 110	-17.879	-22.330	20.685	1.00	19.81	A
ATOM	834	CG2	THR A 110	-15.654	-22.546	19.697	1.00	17.30	A
ATOM	835	C	THR A 110	-18.572	-20.118	19.136	1.00	19.22	A
ATOM	836	O	THR A 110	-19.167	-19.492	20.023	1.00	17.85	A
ATOM	837	N	LEU A 111	-19.124	-20.499	17.991	1.00	18.88	A
ATOM	838	CA	LEU A 111	-20.553	-20.351	17.716	1.00	19.64	A
ATOM	839	CB	LEU A 111	-20.847	-19.228	16.737	1.00	19.79	A
ATOM	840	CG	LEU A 111	-20.773	-17.810	17.316	1.00	19.24	A
ATOM	841	CD1	LEU A 111	-20.926	-16.832	16.218	1.00	19.44	A
ATOM	842	CD2	LEU A 111	-21.882	-17.599	18.408	1.00	20.76	A
ATOM	843	C	LEU A 111	-20.887	-21.715	17.112	1.00	20.43	A
ATOM	844	O	LEU A 111	-20.073	-22.344	16.402	1.00	18.31	A
ATOM	845	N	PRO A 112	-22.085	-22.222	17.394	1.00	19.50	A
ATOM	846	CD	PRO A 112	-23.083	-21.651	18.318	1.00	20.92	A
ATOM	847	CA	PRO A 112	-22.523	-23.525	16.899	1.00	20.93	A
ATOM	848	CB	PRO A 112	-23.959	-23.605	17.391	1.00	22.46	A
ATOM	849	CG	PRO A 112	-23.884	-22.845	18.660	1.00	21.60	A
ATOM	850	C	PRO A 112	-22.421	-23.751	15.398	1.00	20.94	A
ATOM	851	O	PRO A 112	-22.767	-22.888	14.582	1.00	21.16	A
ATOM	852	N	ALA A 113	-21.904	-24.922	15.040	1.00	22.00	A
ATOM	853	CA	ALA A 113	-21.786	-25.266	13.625	1.00	23.34	A
ATOM	854	CB	ALA A 113	-21.161	-26.665	13.485	1.00	22.78	A
ATOM	855	C	ALA A 113	-23.191	-25.235	13.006	1.00	25.52	A
ATOM	856	O	ALA A 113	-23.369	-24.901	11.826	1.00	24.33	A
ATOM	857	N	ALA A 114	-24.191	-25.575	13.812	1.00	26.80	A
ATOM	858	CA	ALA A 114	-25.576	-25.561	13.345	1.00	29.91	A
ATOM	859	CB	ALA A 114	-26.479	-26.091	14.435	1.00	29.86	A
ATOM	860	C	ALA A 114	-26.049	-24.167	12.904	1.00	31.08	A
ATOM	861	O	ALA A 114	-27.019	-24.040	12.146	1.00	32.98	A
ATOM	862	N	ASP A 115	-25.366	-23.127	13.370	1.00	31.48	A
ATOM	863	CA	ASP A 115	-25.706	-21.738	13.046	1.00	30.69	A
ATOM	864	CB	ASP A 115	-25.221	-20.795	14.150	1.00	32.52	A
ATOM	865	CG	ASP A 115	-25.969	-20.954	15.464	1.00	33.04	A

Figure 1 (continued 9)

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ATOM    866  OD1 ASP A 115     -26.756 -21.906  15.653  1.00 34.66      A
ATOM    867  OD2 ASP A 115     -25.737 -20.092  16.336  1.00 36.15      A
ATOM    868  C   ASP A 115     -25.058 -21.240  11.764  1.00 31.41      A
ATOM    869  O   ASP A 115     -25.450 -20.196  11.235  1.00 30.02      A
ATOM    870  N   PHE A 116     -24.038 -21.951  11.286  1.00 30.62      A
ATOM    871  CA  PHE A 116     -23.315 -21.513  10.102  1.00 31.36      A
ATOM    872  CB  PHE A 116     -22.046 -22.362   9.881  1.00 29.27      A
ATOM    873  CG  PHE A 116     -20.991 -21.658   9.069  1.00 27.56      A
ATOM    874  CD1 PHE A 116     -20.203 -20.670   9.641  1.00 27.11      A
ATOM    875  CD2 PHE A 116     -20.805 -21.958   7.721  1.00 27.96      A
ATOM    876  CE1 PHE A 116     -19.246 -19.982   8.889  1.00 28.16      A
ATOM    877  CE2 PHE A 116     -19.855 -21.280   6.963  1.00 28.67      A
ATOM    878  CZ  PHE A 116     -19.071 -20.288   7.546  1.00 29.11      A
ATOM    879  C   PHE A 116     -24.191 -21.561   8.863  1.00 33.68      A
ATOM    880  O   PHE A 116     -24.650 -22.627   8.463  1.00 33.88      A
ATOM    881  N   PRO A 117     -24.425 -20.397   8.238  1.00 36.47      A
ATOM    882  CD  PRO A 117     -23.799 -19.093   8.500  1.00 37.82      A
ATOM    883  CA  PRO A 117     -25.260 -20.325   7.042  1.00 38.24      A
ATOM    884  CB  PRO A 117     -25.299 -18.826   6.721  1.00 38.61      A
ATOM    885  CG  PRO A 117     -24.854 -18.146   8.000  1.00 38.51      A
ATOM    886  C   PRO A 117     -24.580 -21.093   5.941  1.00 39.43      A
ATOM    887  O   PRO A 117     -23.363 -21.079   5.840  1.00 40.03      A
ATOM    888  N   ASN A 118     -25.366 -21.786   5.133  1.00 41.49      A
ATOM    889  CA  ASN A 118     -24.818 -22.514   4.005  1.00 42.60      A
ATOM    890  CB  ASN A 118     -24.654 -23.999   4.334  1.00 45.18      A
ATOM    891  CG  ASN A 118     -25.954 -24.662   4.699  1.00 46.71      A
ATOM    892  OD1 ASN A 118     -26.693 -24.180   5.564  1.00 48.14      A
ATOM    893  ND2 ASN A 118     -26.242 -25.782   4.049  1.00 47.23      A
ATOM    894  C   ASN A 118     -25.787 -22.308   2.856  1.00 42.69      A
ATOM    895  O   ASN A 118     -27.006 -22.231   3.065  1.00 43.09      A
ATOM    896  N   LEU A 119     -25.242 -22.165   1.655  1.00 41.35      A
ATOM    897  CA  LEU A 119     -26.073 -21.954   0.485  1.00 41.09      A
ATOM    898  CB  LEU A 119     -25.208 -21.818  -0.774  1.00 38.77      A
ATOM    899  CG  LEU A 119     -24.451 -20.490  -0.937  1.00 38.25      A
ATOM    900  CD1 LEU A 119     -23.588 -20.520  -2.192  1.00 37.70      A
ATOM    901  CD2 LEU A 119     -25.453 -19.357  -1.028  1.00 36.82      A
ATOM    902  C   LEU A 119     -27.015 -23.132   0.350  1.00 41.13      A
ATOM    903  O   LEU A 119     -26.623 -24.284   0.577  1.00 41.95      A
ATOM    904  N   ASP A 120     -28.266 -22.833   0.011  1.00 41.01      A
ATOM    905  CA  ASP A 120     -29.263 -23.870  -0.171  1.00 41.25      A
ATOM    906  CB  ASP A 120     -30.624 -23.263  -0.503  1.00 42.92      A
ATOM    907  CG  ASP A 120     -31.197 -22.481   0.649  1.00 43.98      A
ATOM    908  OD1 ASP A 120     -31.099 -22.974   1.794  1.00 45.98      A
ATOM    909  OD2 ASP A 120     -31.745 -21.384   0.411  1.00 45.63      A
ATOM    910  C   ASP A 120     -28.824 -24.775  -1.302  1.00 40.45      A
ATOM    911  O   ASP A 120     -28.077 -24.362  -2.197  1.00 40.20      A
ATOM    912  N   ASP A 121     -29.272 -26.018  -1.253  1.00 38.62      A
ATOM    913  CA  ASP A 121     -28.919 -26.947  -2.299  1.00 36.77      A
ATOM    914  CB  ASP A 121     -29.544 -28.319  -2.034  1.00 39.85      A
ATOM    915  CG  ASP A 121     -28.813 -29.091  -0.944  1.00 43.33      A
ATOM    916  OD1 ASP A 121     -27.587 -29.317  -1.094  1.00 44.66      A
ATOM    917  OD2 ASP A 121     -29.460 -29.472   0.059  1.00 45.13      A
ATOM    918  C   ASP A 121     -29.420 -26.365  -3.614  1.00 33.67      A
ATOM    919  O   ASP A 121     -30.401 -25.623  -3.656  1.00 33.57      A
ATOM    920  N   TRP A 122     -28.711 -26.684  -4.681  1.00 30.14      A
ATOM    921  CA  TRP A 122     -29.077 -26.194  -5.992  1.00 25.84      A
ATOM    922  CB  TRP A 122     -28.391 -24.839  -6.253  1.00 24.07      A
ATOM    923  CG  TRP A 122     -26.889 -24.848  -6.119  1.00 21.27      A
ATOM    924  CD2 TRP A 122     -25.938 -24.939  -7.188  1.00 20.32      A
ATOM    925  CE2 TRP A 122     -24.654 -24.929  -6.609  1.00 20.70      A
ATOM    926  CE3 TRP A 122     -26.052 -25.027  -8.580  1.00 17.91      A
ATOM    927  CD1 TRP A 122     -26.160 -24.786  -4.959  1.00 22.23      A
ATOM    928  NE1 TRP A 122     -24.817 -24.832  -5.249  1.00 20.82      A
ATOM    929  CZ2 TRP A 122     -23.486 -25.000  -7.378  1.00 21.15      A
ATOM    930  CZ3 TRP A 122     -24.899 -25.099  -9.351  1.00 19.53      A
ATOM    931  CH2 TRP A 122     -23.621 -25.083  -8.743  1.00 19.91      A
ATOM    932  C   TRP A 122     -28.636 -27.256  -6.992  1.00 25.27      A
ATOM    933  O   TRP A 122     -28.010 -28.255  -6.618  1.00 24.64      A
ATOM    934  N   GLN A 123     -28.965 -27.064  -8.257  1.00 22.99      A
ATOM    935  CA  GLN A 123     -28.612 -28.050  -9.261  1.00 23.31      A
ATOM    936  CB  GLN A 123     -29.882 -28.686  -9.785  1.00 25.63      A
ATOM    937  CG  GLN A 123     -29.649 -30.014 -10.410  1.00 31.98      A
ATOM    938  CD  GLN A 123     -29.414 -31.110  -9.363  1.00 32.90      A
ATOM    939  OE1 GLN A 123     -28.877 -32.157  -9.681  1.00 36.51      A
ATOM    940  NE2 GLN A 123     -29.836 -30.869  -8.109  1.00 33.21      A
ATOM    941  C   GLN A 123     -27.811 -27.488 -10.441  1.00 21.76      A
ATOM    942  O   GLN A 123     -28.179 -26.467 -10.999  1.00 21.19      A
ATOM    943  N   SER A 124     -26.743 -28.163 -10.855  1.00 22.29      A
ATOM    944  CA  SER A 124     -25.993 -27.635 -11.990  1.00 23.13      A
ATOM    945  CB  SER A 124     -24.548 -28.143 -12.016  1.00 26.37      A
ATOM    946  OG  SER A 124     -24.479 -29.416 -12.593  1.00 30.20      A
ATOM    947  C   SER A 124     -26.706 -28.034 -13.274  1.00 22.74      A
ATOM    948  O   SER A 124     -27.311 -29.119 -13.358  1.00 21.31      A
ATOM    949  N   GLU A 125     -26.627 -27.150 -14.265  1.00 22.78      A
ATOM    950  CA  GLU A 125     -27.261 -27.343 -15.553  1.00 23.65      A
ATOM    951  CB  GLU A 125     -28.368 -26.300 -15.707  1.00 26.17      A
ATOM    952  CG  GLU A 125     -29.141 -26.116 -14.428  1.00 30.96      A
ATOM    953  CD  GLU A 125     -30.412 -25.337 -14.617  1.00 34.88      A
ATOM    954  OE1 GLU A 125     -30.408 -24.412 -15.458  1.00 38.83      A
ATOM    955  OE2 GLU A 125     -31.409 -25.650 -13.917  1.00 38.64      A
ATOM    956  C   GLU A 125     -26.274 -27.255 -16.701  1.00 22.71      A
ATOM    957  O   GLU A 125     -26.561 -27.694 -17.806  1.00 22.51      A
ATOM    958  N   VAL A 126     -25.101 -26.692 -16.427  1.00 20.09      A
ATOM    959  CA  VAL A 126     -24.048 -26.531 -17.411  1.00 21.58      A
ATOM    960  CB  VAL A 126     -24.023 -25.055 -17.937  1.00 22.61      A
ATOM    961  CG1 VAL A 126     -23.060 -24.927 -19.077  1.00 25.78      A
ATOM    962  CG2 VAL A 126     -25.433 -24.627 -18.355  1.00 25.22      A
ATOM    963  C   VAL A 126     -22.730 -26.817 -16.729  1.00 19.60      A
ATOM    964  O   VAL A 126     -22.476 -26.270 -15.676  1.00 19.58      A
ATOM    965  N   GLU A 127     -21.898 -27.661 -17.318  1.00 17.89      A
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Figure 1 (continued 10)

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ATOM    966  CA   GLU A 127     -20.602 -27.975 -16.742  1.00 19.23       A
ATOM    967  CB   GLU A 127     -20.643 -29.341 -16.024  1.00 18.90       A
ATOM    968  CG   GLU A 127     -21.759 -29.457 -15.033  1.00 18.41       A
ATOM    969  CD   GLU A 127     -21.797 -30.796 -14.274  1.00 18.10       A
ATOM    970  OE1  GLU A 127     -21.217 -31.797 -14.742  1.00 22.04       A
ATOM    971  OE2  GLU A 127     -22.431 -30.819 -13.209  1.00 19.35       A
ATOM    972  C    GLU A 127     -19.509 -28.013 -17.791  1.00 19.53       A
ATOM    973  O    GLU A 127     -19.741 -28.464 -18.933  1.00 20.65       A
ATOM    974  N    PHE A 128     -18.312 -27.578 -17.403  1.00 17.93       A
ATOM    975  CA   PHE A 128     -17.171 -27.600 -18.304  1.00 18.52       A
ATOM    976  CB   PHE A 128     -17.329 -26.530 -19.409  1.00 19.39       A
ATOM    977  CG   PHE A 128     -17.528 -25.136 -18.866  1.00 18.24       A
ATOM    978  CD1  PHE A 128     -16.423 -24.329 -18.575  1.00 18.53       A
ATOM    979  CD2  PHE A 128     -18.818 -24.640 -18.668  1.00 18.55       A
ATOM    980  CE1  PHE A 128     -16.605 -23.031 -18.044  1.00 18.93       A
ATOM    981  CE2  PHE A 128     -19.014 -23.347 -18.134  1.00 18.45       A
ATOM    982  CZ   PHE A 128     -17.909 -22.541 -17.822  1.00 17.31       A
ATOM    983  C    PHE A 128     -15.900 -27.381 -17.519  1.00 19.63       A
ATOM    984  O    PHE A 128     -15.922 -27.006 -16.335  1.00 16.92       A
ATOM    985  N    THR A 129     -14.785 -27.656 -18.174  1.00 19.01       A
ATOM    986  CA   THR A 129     -13.497 -27.456 -17.561  1.00 21.20       A
ATOM    987  CB   THR A 129     -12.696 -28.761 -17.436  1.00 24.95       A
ATOM    988  OG1  THR A 129     -12.403 -29.263 -18.751  1.00 27.82       A
ATOM    989  CG2  THR A 129     -13.471 -29.800 -16.613  1.00 24.46       A
ATOM    990  C    THR A 129     -12.729 -26.538 -18.479  1.00 21.52       A
ATOM    991  O    THR A 129     -13.035 -26.429 -19.669  1.00 24.36       A
ATOM    992  N    LEU A 130     -11.743 -25.858 -17.923  1.00 21.67       A
ATOM    993  CA   LEU A 130     -10.885 -25.005 -18.716  1.00 21.43       A
ATOM    994  CB   LEU A 130     -11.600 -23.722 -19.161  1.00 21.02       A
ATOM    995  CG   LEU A 130     -11.737 -22.614 -18.130  1.00 21.55       A
ATOM    996  CD1  LEU A 130     -12.246 -21.359 -18.862  1.00 18.68       A
ATOM    997  CD2  LEU A 130     -12.684 -23.045 -17.006  1.00 20.37       A
ATOM    998  C    LEU A 130      -9.666 -24.689 -17.877  1.00 20.77       A
ATOM    999  O    LEU A 130      -9.676 -24.832 -16.645  1.00 21.88       A
ATOM   1000  N    PRO A 131      -8.576 -24.302 -18.535  1.00 21.78       A
ATOM   1001  CD   PRO A 131      -8.433 -24.202 -19.997  1.00 22.11       A
ATOM   1002  CA   PRO A 131      -7.327 -23.970 -17.864  1.00 22.02       A
ATOM   1003  CB   PRO A 131      -6.382 -23.669 -19.023  1.00 21.96       A
ATOM   1004  CG   PRO A 131      -6.975 -24.434 -20.168  1.00 22.46       A
ATOM   1005  C    PRO A 131      -7.468 -22.772 -16.938  1.00 23.06       A
ATOM   1006  O    PRO A 131      -8.194 -21.823 -17.256  1.00 22.79       A
ATOM   1007  N    GLN A 132      -6.767 -22.806 -15.808  1.00 22.91       A
ATOM   1008  CA   GLN A 132      -6.813 -21.686 -14.868  1.00 23.70       A
ATOM   1009  CB   GLN A 132      -5.881 -21.922 -13.678  1.00 25.71       A
ATOM   1010  CG   GLN A 132      -6.311 -23.098 -12.821  1.00 29.70       A
ATOM   1011  CD   GLN A 132      -5.450 -23.279 -11.576  1.00 32.46       A
ATOM   1012  OE1  GLN A 132      -5.308 -22.365 -10.762  1.00 32.13       A
ATOM   1013  NE2  GLN A 132      -4.878 -24.477 -11.425  1.00 33.56       A
ATOM   1014  C    GLN A 132      -6.394 -20.419 -15.581  1.00 22.79       A
ATOM   1015  O    GLN A 132      -6.999 -19.368 -15.380  1.00 21.02       A
ATOM   1016  N    ALA A 133      -5.375 -20.517 -16.424  1.00 21.06       A
ATOM   1017  CA   ALA A 133      -4.897 -19.337 -17.154  1.00 22.13       A
ATOM   1018  CB   ALA A 133      -3.624 -19.681 -17.935  1.00 22.47       A
ATOM   1019  C    ALA A 133      -5.942 -18.757 -18.098  1.00 20.39       A
ATOM   1020  O    ALA A 133      -5.932 -17.559 -18.361  1.00 21.36       A
ATOM   1021  N    THR A 134      -6.833 -19.590 -18.630  1.00 18.88       A
ATOM   1022  CA   THR A 134      -7.853 -19.085 -19.549  1.00 18.20       A
ATOM   1023  CB   THR A 134      -8.512 -20.254 -20.296  1.00 19.77       A
ATOM   1024  OG1  THR A 134      -7.498 -20.911 -21.092  1.00 19.04       A
ATOM   1025  CG2  THR A 134      -9.594 -19.776 -21.214  1.00 18.65       A
ATOM   1026  C    THR A 134      -8.885 -18.288 -18.773  1.00 17.20       A
ATOM   1027  O    THR A 134      -9.341 -17.214 -19.190  1.00 16.08       A
ATOM   1028  N    MET A 135      -9.260 -18.827 -17.627  1.00 17.79       A
ATOM   1029  CA   MET A 135     -10.237 -18.138 -16.786  1.00 18.34       A
ATOM   1030  CB   MET A 135     -10.612 -19.011 -15.579  1.00 18.90       A
ATOM   1031  CG   MET A 135     -11.596 -18.329 -14.623  1.00 21.27       A
ATOM   1032  SD   MET A 135     -13.215 -17.944 -15.348  1.00 25.97       A
ATOM   1033  CE   MET A 135     -13.884 -19.343 -15.539  1.00 21.37       A
ATOM   1034  C    MET A 135      -9.677 -16.800 -16.311  1.00 18.69       A
ATOM   1035  O    MET A 135     -10.386 -15.793 -16.327  1.00 17.86       A
ATOM   1036  N    LYS A 136      -8.409 -16.776 -15.890  1.00 18.69       A
ATOM   1037  CA   LYS A 136      -7.754 -15.553 -15.443  1.00 20.30       A
ATOM   1038  CB   LYS A 136      -6.302 -15.835 -15.024  1.00 23.59       A
ATOM   1039  CG   LYS A 136      -5.351 -14.628 -15.146  1.00 28.29       A
ATOM   1040  CD   LYS A 136      -3.863 -15.004 -14.987  1.00 31.41       A
ATOM   1041  CE   LYS A 136      -3.406 -16.112 -15.975  1.00 35.30       A
ATOM   1042  NZ   LYS A 136      -3.714 -15.883 -17.445  1.00 35.62       A
ATOM   1043  C    LYS A 136      -7.752 -14.531 -16.578  1.00 19.86       A
ATOM   1044  O    LYS A 136      -8.004 -13.352 -16.364  1.00 20.49       A
ATOM   1045  N    ARG A 137      -7.445 -14.988 -17.786  1.00 17.95       A
ATOM   1046  CA   ARG A 137      -7.423 -14.094 -18.915  1.00 16.91       A
ATOM   1047  CB   ARG A 137      -6.931 -14.844 -20.152  1.00 20.63       A
ATOM   1048  CG   ARG A 137      -6.418 -13.923 -21.256  1.00 27.85       A
ATOM   1049  CD   ARG A 137      -7.457 -13.620 -22.307  1.00 32.60       A
ATOM   1050  NE   ARG A 137      -7.054 -12.470 -23.126  1.00 38.30       A
ATOM   1051  CZ   ARG A 137      -7.656 -12.105 -24.254  1.00 39.88       A
ATOM   1052  NH1  ARG A 137      -8.682 -12.806 -24.718  1.00 42.58       A
ATOM   1053  NH2  ARG A 137      -7.255 -11.029 -24.915  1.00 38.76       A
ATOM   1054  C    ARG A 137      -8.819 -13.504 -19.171  1.00 16.74       A
ATOM   1055  O    ARG A 137      -8.950 -12.317 -19.436  1.00 16.26       A
ATOM   1056  N    LEU A 138      -9.846 -14.333 -19.081  1.00 13.43       A
ATOM   1057  CA   LEU A 138     -11.202 -13.848 -19.338  1.00 13.64       A
ATOM   1058  CB   LEU A 138     -12.201 -15.020 -19.290  1.00 14.57       A
ATOM   1059  CG   LEU A 138     -12.160 -15.924 -20.526  1.00 14.17       A
ATOM   1060  CD1  LEU A 138     -12.888 -17.223 -20.219  1.00 17.01       A
ATOM   1061  CD2  LEU A 138     -12.794 -15.194 -21.734  1.00 15.21       A
ATOM   1062  C    LEU A 138     -11.604 -12.799 -18.341  1.00 13.26       A
ATOM   1063  O    LEU A 138     -12.232 -11.788 -18.700  1.00 13.04       A
ATOM   1064  N    ILE A 139     -11.269 -13.036 -17.073  1.00 13.36       A
ATOM   1065  CA   ILE A 139     -11.642 -12.066 -16.049  1.00 14.01       A
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Figure 1 (continued 11)

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ATOM   1066  CB   ILE A 139     -11.574 -12.711 -14.631  1.00 14.80          A
ATOM   1067  CG2  ILE A 139     -11.749 -11.612 -13.554  1.00 14.76          A
ATOM   1068  CG1  ILE A 139     -12.657 -13.793 -14.526  1.00 14.38          A
ATOM   1069  CD1  ILE A 139     -12.522 -14.700 -13.259  1.00 15.70          A
ATOM   1070  C    ILE A 139     -10.828 -10.782 -16.115  1.00 15.36          A
ATOM   1071  O    ILE A 139     -11.403  -9.681 -16.129  1.00 15.94          A
ATOM   1072  N    GLU A 140      -9.500 -10.891 -16.185  1.00 14.35          A
ATOM   1073  CA   GLU A 140      -8.663  -9.698 -16.254  1.00 16.18          A
ATOM   1074  CB   GLU A 140      -7.175 -10.107 -16.250  1.00 18.11          A
ATOM   1075  CG   GLU A 140      -6.708 -10.696 -14.927  1.00 24.32          A
ATOM   1076  CD   GLU A 140      -5.209 -11.032 -14.909  1.00 29.34          A
ATOM   1077  OE1  GLU A 140      -4.642 -11.276 -15.995  1.00 31.06          A
ATOM   1078  OE2  GLU A 140      -4.606 -11.069 -13.804  1.00 33.19          A
ATOM   1079  C    GLU A 140      -8.955  -8.832 -17.481  1.00 15.66          A
ATOM   1080  O    GLU A 140      -8.774  -7.613 -17.452  1.00 16.06          A
ATOM   1081  N    ALA A 141      -9.428  -9.458 -18.547  1.00 14.10          A
ATOM   1082  CA   ALA A 141      -9.690  -8.725 -19.785  1.00 12.46          A
ATOM   1083  CB   ALA A 141      -9.921  -9.712 -20.945  1.00 16.01          A
ATOM   1084  C    ALA A 141     -10.893  -7.796 -19.666  1.00 13.15          A
ATOM   1085  O    ALA A 141     -11.005  -6.834 -20.422  1.00 12.75          A
ATOM   1086  N    THR A 142     -11.771  -8.088 -18.726  1.00 12.50          A
ATOM   1087  CA   THR A 142     -13.017  -7.313 -18.635  1.00 10.74          A
ATOM   1088  CB   THR A 142     -14.234  -8.165 -19.093  1.00 11.13          A
ATOM   1089  OG1  THR A 142     -14.408  -9.249 -18.173  1.00 15.23          A
ATOM   1090  CG2  THR A 142     -14.000  -8.750 -20.499  1.00 11.74          A
ATOM   1091  C    THR A 142     -13.397  -6.766 -17.277  1.00 13.68          A
ATOM   1092  O    THR A 142     -14.208  -5.849 -17.229  1.00 12.84          A
ATOM   1093  N    GLN A 143     -12.824  -7.279 -16.193  1.00 12.98          A
ATOM   1094  CA   GLN A 143     -13.218  -6.886 -14.832  1.00 14.94          A
ATOM   1095  CB   GLN A 143     -12.264  -7.548 -13.841  1.00 17.55          A
ATOM   1096  CG   GLN A 143     -12.686  -7.401 -12.422  1.00 23.99          A
ATOM   1097  CD   GLN A 143     -11.760  -8.145 -11.481  1.00 27.58          A
ATOM   1098  OE1  GLN A 143     -12.121  -8.446 -10.332  1.00 31.11          A
ATOM   1099  NE2  GLN A 143     -10.561  -8.434 -11.956  1.00 27.03          A
ATOM   1100  C    GLN A 143     -13.311  -5.398 -14.533  1.00 14.23          A
ATOM   1101  O    GLN A 143     -14.235  -4.946 -13.808  1.00 15.54          A
ATOM   1102  N    PHE A 144     -12.372  -4.641 -15.073  1.00 14.47          A
ATOM   1103  CA   PHE A 144     -12.312  -3.206 -14.848  1.00 14.06          A
ATOM   1104  CB   PHE A 144     -11.028  -2.636 -15.430  1.00 13.76          A
ATOM   1105  CG   PHE A 144     -11.014  -2.621 -16.924  1.00 16.11          A
ATOM   1106  CD1  PHE A 144     -10.537  -3.718 -17.656  1.00 14.91          A
ATOM   1107  CD2  PHE A 144     -11.524  -1.510 -17.611  1.00 15.82          A
ATOM   1108  CE1  PHE A 144     -10.567  -3.701 -19.064  1.00 15.95          A
ATOM   1109  CE2  PHE A 144     -11.558  -1.484 -19.000  1.00 16.83          A
ATOM   1110  CZ   PHE A 144     -11.080  -2.579 -19.730  1.00 18.10          A
ATOM   1111  C    PHE A 144     -13.503  -2.424 -15.388  1.00 15.25          A
ATOM   1112  O    PHE A 144     -13.727  -1.296 -14.957  1.00 14.82          A
ATOM   1113  N    SER A 145     -14.268  -3.019 -16.306  1.00 13.80          A
ATOM   1114  CA   SER A 145     -15.442  -2.334 -16.873  1.00 14.34          A
ATOM   1115  CB   SER A 145     -15.637  -2.720 -18.328  1.00 15.77          A
ATOM   1116  OG   SER A 145     -14.570  -2.200 -19.120  1.00 16.45          A
ATOM   1117  C    SER A 145     -16.737  -2.587 -16.121  1.00 15.00          A
ATOM   1118  O    SER A 145     -17.787  -2.069 -16.526  1.00 15.49          A
ATOM   1119  N    MET A 146     -16.699  -3.407 -15.084  1.00 15.16          A
ATOM   1120  CA   MET A 146     -17.917  -3.660 -14.288  1.00 15.61          A
ATOM   1121  CB   MET A 146     -17.677  -4.746 -13.224  1.00 16.31          A
ATOM   1122  CG   MET A 146     -17.414  -6.142 -13.771  1.00 16.90          A
ATOM   1123  SD   MET A 146     -17.264  -7.426 -12.423  1.00 20.35          A
ATOM   1124  CE   MET A 146     -15.868  -6.822 -11.667  1.00 18.34          A
ATOM   1125  C    MET A 146     -18.290  -2.364 -13.546  1.00 17.87          A
ATOM   1126  O    MET A 146     -17.436  -1.571 -13.177  1.00 17.71          A
ATOM   1127  N    ALA A 147     -19.584  -2.171 -13.302  1.00 18.85          A
ATOM   1128  CA   ALA A 147     -20.000  -0.987 -12.561  1.00 22.61          A
ATOM   1129  CB   ALA A 147     -21.514  -0.786 -12.718  1.00 20.80          A
ATOM   1130  C    ALA A 147     -19.666  -1.181 -11.088  1.00 25.26          A
ATOM   1131  O    ALA A 147     -19.455  -2.315 -10.624  1.00 25.14          A
ATOM   1132  N    HIS A 148     -19.654  -0.068 -10.359  1.00 29.57          A
ATOM   1133  CA   HIS A 148     -19.407  -0.078  -8.916  1.00 32.55          A
ATOM   1134  CB   HIS A 148     -18.185   0.755  -8.530  1.00 35.09          A
ATOM   1135  CG   HIS A 148     -16.886   0.218  -9.025  1.00 38.05        } A
ATOM   1136  CD2  HIS A 148     -15.868  -0.390  -8.368  1.00 38.84          A
ATOM   1137  ND1  HIS A 148     -16.477   0.347 -10.336  1.00 39.33          A
ATOM   1138  CE1  HIS A 148     -15.259  -0.151 -10.463  1.00 39.25          A
ATOM   1139  NE2  HIS A 148     -14.867  -0.603  -9.284  1.00 39.69          A
ATOM   1140  C    HIS A 148     -20.588   0.578  -8.210  1.00 32.61          A
ATOM   1141  O    HIS A 148     -20.810   1.781  -8.365  1.00 33.21          A
ATOM   1142  N    GLN A 149     -21.326  -0.203  -7.436  1.00 32.56          A
ATOM   1143  CA   GLN A 149     -22.449   0.309  -6.663  1.00 33.37          A
ATOM   1144  CB   GLN A 149     -21.922   1.256  -5.575  1.00 35.74          A
ATOM   1145  CG   GLN A 149     -20.875   0.614  -4.657  1.00 39.57          A
ATOM   1146  CD   GLN A 149     -20.358   1.564  -3.573  1.00 41.69          A
ATOM   1147  OE1  GLN A 149     -21.099   2.399  -3.059  1.00 42.95          A
ATOM   1148  NE2  GLN A 149     -19.084   1.420  -3.214  1.00 41.85          A
ATOM   1149  C    GLN A 149     -23.529   1.008  -7.486  1.00 32.00          A
ATOM   1150  O    GLN A 149     -24.177   1.957  -7.016  1.00 32.50          A
ATOM   1151  N    ASP A 150     -23.742   0.538  -8.704  1.00 29.36          A
ATOM   1152  CA   ASP A 150     -24.772   1.110  -9.560  1.00 27.85          A
ATOM   1153  CB   ASP A 150     -24.532   0.681 -11.006  1.00 26.70          A
ATOM   1154  CG   ASP A 150     -25.318   1.510 -12.007  1.00 27.39          A
ATOM   1155  OD1  ASP A 150     -24.695   2.262 -12.791  1.00 27.00          A
ATOM   1156  OD2  ASP A 150     -26.558   1.410 -12.017  1.00 26.08          A
ATOM   1157  C    ASP A 150     -26.143   0.601  -9.093  1.00 27.65          A
ATOM   1158  O    ASP A 150     -26.291  -0.565  -8.720  1.00 27.65          A
ATOM   1159  N    VAL A 151     -27.148   1.475  -9.100  1.00 28.95          A
ATOM   1160  CA   VAL A 151     -28.495   1.080  -8.702  1.00 30.15          A
ATOM   1161  CB   VAL A 151     -29.462   2.274  -8.840  1.00 30.10          A
ATOM   1162  CG1  VAL A 151     -30.898   1.825  -8.593  1.00 33.02          A
ATOM   1163  CG2  VAL A 151     -29.065   3.354  -7.856  1.00 32.71          A
ATOM   1164  C    VAL A 151     -28.985  -0.099  -9.552  1.00 29.78          A
ATOM   1165  O    VAL A 151     -29.860  -0.858  -9.137  1.00 29.45          A
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Figure 1 (continued 12)

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ATOM   1166   N    ARG A 152    -28.431   -0.251  -10.752  1.00  29.05        A
ATOM   1167   CA   ARG A 152    -28.804   -1.379  -11.596  1.00  27.89        A
ATOM   1168   CB   ARG A 152    -28.634   -1.019  -13.069  1.00  26.83        A
ATOM   1169   CG   ARG A 152    -29.512    0.180  -13.508  1.00  26.45        A
ATOM   1170   CD   ARG A 152    -29.040    0.760  -14.836  1.00  26.01        A
ATOM   1171   NE   ARG A 152    -27.778    1.484  -14.686  1.00  24.71        A
ATOM   1172   CZ   ARG A 152    -27.089    2.005  -15.701  1.00  21.61        A
ATOM   1173   NH1  ARG A 152    -27.529    1.890  -16.950  1.00  23.37        A
ATOM   1174   NH2  ARG A 152    -25.947    2.627  -15.469  1.00  22.47        A
ATOM   1175   C    ARG A 152    -27.813   -2.455  -11.176  1.00  27.21        A
ATOM   1176   O    ARG A 152    -26.719   -2.545  -11.722  1.00  24.79        A
ATOM   1177   N    TYR A 153    -28.197   -3.226  -10.163  1.00  27.89        A
ATOM   1178   CA   TYR A 153    -27.379   -4.284   -9.588  1.00  28.26        A
ATOM   1179   CB   TYR A 153    -28.198   -5.074   -8.566  1.00  32.74        A
ATOM   1180   CG   TYR A 153    -29.435   -5.685   -9.190  1.00  36.87        A
ATOM   1181   CD1  TYR A 153    -30.400   -4.879   -9.808  1.00  39.09        A
ATOM   1182   CE1  TYR A 153    -31.510   -5.434  -10.445  1.00  41.32        A
ATOM   1183   CD2  TYR A 153    -29.620   -7.069   -9.212  1.00  38.75        A
ATOM   1184   CE2  TYR A 153    -30.734   -7.637   -9.839  1.00  41.39        A
ATOM   1185   CZ   TYR A 153    -31.670   -6.814  -10.459  1.00  41.82        A
ATOM   1186   OH   TYR A 153    -32.744   -7.366  -11.122  1.00  43.97        A
ATOM   1187   C    TYR A 153    -26.802   -5.265  -10.594  1.00  25.95        A
ATOM   1188   O    TYR A 153    -25.720   -5.798  -10.355  1.00  25.41        A
ATOM   1189   N    TYR A 154    -27.521   -5.522  -11.683  1.00  24.27        A
ATOM   1190   CA   TYR A 154    -27.038   -6.490  -12.683  1.00  24.02        A
ATOM   1191   CB   TYR A 154    -28.138   -6.822  -13.697  1.00  24.80        A
ATOM   1192   CG   TYR A 154    -28.704   -5.632  -14.441  1.00  26.56        A
ATOM   1193   CD1  TYR A 154    -28.095   -5.150  -15.603  1.00  26.67        A
ATOM   1194   CE1  TYR A 154    -28.609   -4.046  -16.280  1.00  28.56        A
ATOM   1195   CD2  TYR A 154    -29.841   -4.982  -13.969  1.00  27.71        A
ATOM   1196   CE2  TYR A 154    -30.366   -3.868  -14.636  1.00  28.26        A
ATOM   1197   CZ   TYR A 154    -29.745   -3.411  -15.789  1.00  29.38        A
ATOM   1198   OH   TYR A 154    -30.269   -2.332  -16.463  1.00  31.98        A
ATOM   1199   C    TYR A 154    -25.786   -5.988  -13.410  1.00  23.05        A
ATOM   1200   O    TYR A 154    -25.156   -6.778  -14.135  1.00  24.65        A
ATOM   1201   N    LEU A 155    -25.433   -4.709  -13.249  1.00  19.62        A
ATOM   1202   CA   LEU A 155    -24.215   -4.190  -13.884  1.00  18.55        A
ATOM   1203   CB   LEU A 155    -24.397   -2.720  -14.330  1.00  18.29        A
ATOM   1204   CG   LEU A 155    -25.393   -2.508  -15.470  1.00  18.19        A
ATOM   1205   CD1  LEU A 155    -25.430   -1.025  -15.872  1.00  20.01        A
ATOM   1206   CD2  LEU A 155    -24.986   -3.351  -16.652  1.00  17.70        A
ATOM   1207   C    LEU A 155    -23.029   -4.270  -12.926  1.00  18.16        A
ATOM   1208   O    LEU A 155    -21.890   -4.047  -13.335  1.00  17.47        A
ATOM   1209   N    ASN A 156    -23.299   -4.538  -11.648  1.00  19.44        A
ATOM   1210   CA   ASN A 156    -22.258   -4.646  -10.622  1.00  19.29        A
ATOM   1211   CB   ASN A 156    -22.776   -4.318   -9.225  1.00  20.80        A
ATOM   1212   CG   ASN A 156    -23.318   -2.927   -9.107  1.00  21.25        A
ATOM   1213   OD1  ASN A 156    -24.221   -2.673   -8.287  1.00  24.83        A
ATOM   1214   ND2  ASN A 156    -22.777   -2.010   -9.887  1.00  16.70        A
ATOM   1215   C    ASN A 156    -21.821   -6.113  -10.587  1.00  19.89        A
ATOM   1216   O    ASN A 156    -21.828   -6.805   -9.535  1.00  23.37        A
ATOM   1217   N    GLY A 157    -21.518   -6.613  -11.753  1.00  17.85        A
ATOM   1218   CA   GLY A 157    -21.070   -7.981  -11.823  1.00  16.12        A
ATOM   1219   C    GLY A 157    -20.565   -8.215  -13.217  1.00  14.85        A
ATOM   1220   O    GLY A 157    -20.399   -7.275  -13.993  1.00  15.61        A
ATOM   1221   N    MET A 158    -20.343   -9.485  -13.544  1.00  13.48        A
ATOM   1222   CA   MET A 158    -19.800   -9.852  -14.842  1.00  13.97        A
ATOM   1223   CB   MET A 158    -18.349  -10.347  -14.646  1.00  13.51        A
ATOM   1224   CG   MET A 158    -17.648  -10.766  -15.928  1.00  12.71        A
ATOM   1225   SD   MET A 158    -15.937  -11.277  -15.551  1.00  12.75        A
ATOM   1226   CE   MET A 158    -15.144   -9.642  -15.273  1.00  14.07        A
ATOM   1227   C    MET A 158    -20.622  -10.936  -15.511  1.00  12.85        A
ATOM   1228   O    MET A 158    -20.950  -11.942  -14.890  1.00  12.99        A
ATOM   1229   N    LEU A 159    -20.941  -10.757  -16.787  1.00  11.15        A
ATOM   1230   CA   LEU A 159    -21.692  -11.772  -17.517  1.00  12.65        A
ATOM   1231   CB   LEU A 159    -22.302  -11.197  -18.799  1.00  14.78        A
ATOM   1232   CG   LEU A 159    -23.251  -12.145  -19.553  1.00  16.09        A
ATOM   1233   CD1  LEU A 159    -24.545  -12.193  -18.732  1.00  16.30        A
ATOM   1234   CD2  LEU A 159    -23.582  -11.680  -20.975  1.00  17.74        A
ATOM   1235   C    LEU A 159    -20.737  -12.884  -17.923  1.00  13.59        A
ATOM   1236   O    LEU A 159    -19.642  -12.598  -18.386  1.00  12.32        A
ATOM   1237   N    PHE A 160    -21.138  -14.119  -17.652  1.00  13.23        A
ATOM   1238   CA   PHE A 160    -20.369  -15.298  -18.110  1.00  13.78        A
ATOM   1239   CB   PHE A 160    -20.017  -16.243  -16.972  1.00  15.17        A
ATOM   1240   CG   PHE A 160    -18.810  -15.822  -16.206  1.00  15.50        A
ATOM   1241   CD1  PHE A 160    -18.845  -14.708  -15.386  1.00  16.70        A
ATOM   1242   CD2  PHE A 160    -17.619  -16.528  -16.340  1.00  20.57        A
ATOM   1243   CE1  PHE A 160    -17.690  -14.301  -14.696  1.00  15.09        A
ATOM   1244   CE2  PHE A 160    -16.473  -16.129  -15.664  1.00  21.51        A
ATOM   1245   CZ   PHE A 160    -16.516  -15.010  -14.837  1.00  19.20        A
ATOM   1246   C    PHE A 160    -21.324  -15.985  -19.078  1.00  14.91        A
ATOM   1247   O    PHE A 160    -22.457  -16.356  -18.712  1.00  14.88        A
ATOM   1248   N    GLU A 161    -20.883  -16.155  -20.326  1.00  14.48        A
ATOM   1249   CA   GLU A 161    -21.732  -16.732  -21.343  1.00  15.81        A
ATOM   1250   CB   GLU A 161    -22.136  -15.629  -22.347  1.00  17.40        A
ATOM   1251   CG   GLU A 161    -22.921  -16.096  -23.576  1.00  21.38        A
ATOM   1252   CD   GLU A 161    -23.306  -14.959  -24.539  1.00  25.94        A
ATOM   1253   OE1  GLU A 161    -22.630  -13.893  -24.551  1.00  23.68        A
ATOM   1254   OE2  GLU A 161    -24.296  -15.148  -25.306  1.00  27.60        A
ATOM   1255   C    GLU A 161    -21.042  -17.858  -22.070  1.00  16.27        A
ATOM   1256   O    GLU A 161    -19.852  -17.753  -22.420  1.00  16.32        A
ATOM   1257   N    THR A 162    -21.785  -18.939  -22.275  1.00  16.15        A
ATOM   1258   CA   THR A 162    -21.255  -20.072  -23.043  1.00  17.00        A
ATOM   1259   CB   THR A 162    -21.579  -21.418  -22.376  1.00  15.79        A
ATOM   1260   OG1  THR A 162    -22.976  -21.471  -22.079  1.00  17.17        A
ATOM   1261   CG2  THR A 162    -20.777  -21.587  -21.073  1.00  17.18        A
ATOM   1262   C    THR A 162    -21.943  -20.022  -24.408  1.00  16.86        A
ATOM   1263   O    THR A 162    -23.133  -19.814  -24.498  1.00  17.96        A
ATOM   1264   N    GLU A 163    -21.184  -20.213  -25.473  1.00  19.48        A
ATOM   1265   CA   GLU A 163    -21.770  -20.170  -26.807  1.00  20.26        A
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Figure 1 (continued 13)

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ATOM   1266  CB  GLU A 163   -21.892 -18.717 -27.287  1.00 21.73      A
ATOM   1267  CG  GLU A 163   -22.630 -18.615 -28.630  1.00 25.04      A
ATOM   1268  CD  GLU A 163   -22.892 -17.188 -29.043  1.00 28.71      A
ATOM   1269  OE1 GLU A 163   -22.046 -16.326 -28.755  1.00 29.00      A
ATOM   1270  OE2 GLU A 163   -23.937 -16.925 -29.672  1.00 33.20      A
ATOM   1271  C   GLU A 163   -20.857 -20.965 -27.717  1.00 20.58      A
ATOM   1272  O   GLU A 163   -19.670 -20.671 -27.849  1.00 19.51      A
ATOM   1273  N   GLY A 164   -21.427 -21.985 -28.336  1.00 21.25      A
ATOM   1274  CA  GLY A 164   -20.643 -22.834 -29.208  1.00 23.06      A
ATOM   1275  C   GLY A 164   -19.570 -23.516 -28.381  1.00 22.55      A
ATOM   1276  O   GLY A 164   -19.860 -24.269 -27.441  1.00 23.22      A
ATOM   1277  N   GLU A 165   -18.323 -23.232 -28.699  1.00 22.46      A
ATOM   1278  CA  GLU A 165   -17.233 -23.835 -27.965  1.00 21.86      A
ATOM   1279  CB  GLU A 165   -16.276 -24.498 -28.948  1.00 26.05      A
ATOM   1280  CG  GLU A 165   -15.133 -25.183 -28.299  1.00 31.89      A
ATOM   1281  CD  GLU A 165   -13.996 -25.386 -29.268  1.00 32.82      A
ATOM   1282  OE1 GLU A 165   -14.228 -26.054 -30.316  1.00 35.85      A
ATOM   1283  OE2 GLU A 165   -12.891 -24.872 -28.983  1.00 32.38      A
ATOM   1284  C   GLU A 165   -16.492 -22.792 -27.122  1.00 20.54      A
ATOM   1285  O   GLU A 165   -15.403 -23.031 -26.629  1.00 21.57      A
ATOM   1286  N   GLU A 166   -17.101 -21.632 -26.932  1.00 18.84      A
ATOM   1287  CA  GLU A 166   -16.419 -20.588 -26.183  1.00 18.69      A
ATOM   1288  CB  GLU A 166   -16.291 -19.332 -27.036  1.00 20.53      A
ATOM   1289  CG  GLU A 166   -15.371 -19.476 -28.244  1.00 25.65      A
ATOM   1290  CD  GLU A 166   -15.124 -18.128 -28.875  1.00 29.36      A
ATOM   1291  OE1 GLU A 166   -16.106 -17.495 -29.317  1.00 29.76      A
ATOM   1292  OE2 GLU A 166   -13.953 -17.697 -28.911  1.00 32.95      A
ATOM   1293  C   GLU A 166   -17.075 -20.149 -24.882  1.00 16.09      A
ATOM   1294  O   GLU A 166   -18.281 -20.299 -24.699  1.00 17.27      A
ATOM   1295  N   LEU A 167   -16.226 -19.667 -23.984  1.00 16.29      A
ATOM   1296  CA  LEU A 167   -16.685 -19.074 -22.722  1.00 14.08      A
ATOM   1297  CB  LEU A 167   -15.916 -19.586 -21.510  1.00 14.28      A
ATOM   1298  CG  LEU A 167   -16.345 -18.898 -20.199  1.00 14.34      A
ATOM   1299  CD1 LEU A 167   -17.852 -19.118 -19.991  1.00 15.20      A
ATOM   1300  CD2 LEU A 167   -15.572 -19.425 -18.995  1.00 15.60      A
ATOM   1301  C   LEU A 167   -16.356 -17.589 -22.956  1.00 14.38      A
ATOM   1302  O   LEU A 167   -15.249 -17.243 -23.413  1.00 14.90      A
ATOM   1303  N   ARG A 168   -17.314 -16.720 -22.632  1.00 13.15      A
ATOM   1304  CA  ARG A 168   -17.142 -15.283 -22.858  1.00 13.65      A
ATOM   1305  CB  ARG A 168   -18.109 -14.851 -23.974  1.00 14.89      A
ATOM   1306  CG  ARG A 168   -18.286 -13.333 -24.147  1.00 14.54      A
ATOM   1307  CD  ARG A 168   -19.316 -13.059 -25.217  1.00 16.30      A
ATOM   1308  NE  ARG A 168   -18.918 -13.676 -26.473  1.00 19.44      A
ATOM   1309  CZ  ARG A 168   -19.627 -14.584 -27.139  1.00 21.39      A
ATOM   1310  NH1 ARG A 168   -20.793 -15.006 -26.690  1.00 22.67      A
ATOM   1311  NH2 ARG A 168   -19.147 -15.073 -28.265  1.00 25.38      A
ATOM   1312  C   ARG A 168   -17.509 -14.523 -21.605  1.00 13.95      A
ATOM   1313  O   ARG A 168   -18.425 -14.932 -20.873  1.00 14.10      A
ATOM   1314  N   THR A 169   -16.794 -13.431 -21.351  1.00 12.43      A
ATOM   1315  CA  THR A 169   -17.153 -12.587 -20.230  1.00 10.45      A
ATOM   1316  CB  THR A 169   -16.053 -12.425 -19.186  1.00 12.78      A
ATOM   1317  OG1 THR A 169   -14.844 -11.981 -19.830  1.00 14.14      A
ATOM   1318  CG2 THR A 169   -15.808 -13.743 -18.422  1.00 11.68      A
ATOM   1319  C   THR A 169   -17.469 -11.219 -20.825  1.00 11.09      A
ATOM   1320  O   THR A 169   -16.932 -10.824 -21.853  1.00 10.97      A
ATOM   1321  N   VAL A 170   -18.421 -10.537 -20.198  1.00 10.12      A
ATOM   1322  CA  VAL A 170   -18.803  -9.205 -20.645  1.00 10.95      A
ATOM   1323  CB  VAL A 170   -20.166  -9.186 -21.384  1.00 10.17      A
ATOM   1324  CG1 VAL A 170   -20.344  -7.769 -22.015  1.00 11.54      A
ATOM   1325  CG2 VAL A 170   -20.197 -10.227 -22.491  1.00 13.32      A
ATOM   1326  C   VAL A 170   -18.967  -8.359 -19.376  1.00 10.18      A
ATOM   1327  O   VAL A 170   -19.500  -8.824 -18.361  1.00 13.17      A
ATOM   1328  N   ALA A 171   -18.471  -7.118 -19.426  1.00 11.08      A
ATOM   1329  CA  ALA A 171   -18.650  -6.212 -18.310  1.00 10.99      A
ATOM   1330  CB  ALA A 171   -17.451  -6.224 -17.401  1.00 12.41      A
ATOM   1331  C   ALA A 171   -18.898  -4.807 -18.854  1.00 12.83      A
ATOM   1332  O   ALA A 171   -18.353  -4.409 -19.875  1.00 13.33      A
ATOM   1333  N   THR A 172   -19.788  -4.091 -18.193  1.00 11.14      A
ATOM   1334  CA  THR A 172   -20.092  -2.723 -18.627  1.00 12.97      A
ATOM   1335  CB  THR A 172   -21.046  -2.669 -19.850  1.00 16.11      A
ATOM   1336  OG1 THR A 172   -21.222  -1.284 -20.236  1.00 15.65      A
ATOM   1337  CG2 THR A 172   -22.435  -3.271 -19.520  1.00 15.53      A
ATOM   1338  C   THR A 172   -20.697  -1.934 -17.486  1.00 13.38      A
ATOM   1339  O   THR A 172   -21.347  -2.484 -16.592  1.00 13.88      A
ATOM   1340  N   ASP A 173   -20.455  -0.624 -17.525  1.00 13.39      A
ATOM   1341  CA  ASP A 173   -20.994   0.264 -16.494  1.00 15.62      A
ATOM   1342  CB  ASP A 173   -19.864  -0.956 -15.731  1.00 16.03      A
ATOM   1343  CG  ASP A 173   -18.990   1.833 -16.625  1.00 16.32      A
ATOM   1344  OD1 ASP A 173   -19.273   1.986 -17.831  1.00 15.70      A
ATOM   1345  OD2 ASP A 173   -18.005   2.370 -16.079  1.00 18.84      A
ATOM   1346  C   ASP A 173   -21.867   1.310 -17.164  1.00 16.64      A
ATOM   1347  O   ASP A 173   -22.214   2.322 -16.530  1.00 19.53      A
ATOM   1348  N   GLY A 174   -22.187   1.083 -18.436  1.00 16.21      A
ATOM   1349  CA  GLY A 174   -23.039   2.014 -19.178  1.00 18.97      A
ATOM   1350  C   GLY A 174   -22.302   3.071 -19.977  1.00 19.77      A
ATOM   1351  O   GLY A 174   -22.884   3.728 -20.860  1.00 21.66      A
ATOM   1352  N   HIS A 175   -21.023   3.258 -19.655  1.00 18.37      A
ATOM   1353  CA  HIS A 175   -20.162   4.210 -20.370  1.00 19.07      A
ATOM   1354  CB  HIS A 175   -19.434   5.082 -19.384  1.00 21.34      A
ATOM   1355  CG  HIS A 175   -20.339   5.944 -18.578  1.00 28.96      A
ATOM   1356  CD2 HIS A 175   -20.783   5.827 -17.305  1.00 31.83      A
ATOM   1357  ND1 HIS A 175   -21.007   7.017 -19.126  1.00 30.11      A
ATOM   1358  CE1 HIS A 175   -21.828   7.524 -18.225  1.00 30.90      A
ATOM   1359  NE2 HIS A 175   -21.713   6.820 -17.111  1.00 34.27      A
ATOM   1360  C   HIS A 175   -19.189   3.501 -21.254  1.00 17.40      A
ATOM   1361  O   HIS A 175   -18.861   3.970 -22.340  1.00 18.83      A
ATOM   1362  N   ARG A 176   -18.663   2.385 -20.755  1.00 15.38      A
ATOM   1363  CA  ARG A 176   -17.713   1.611 -21.529  1.00 14.12      A
ATOM   1364  CB  ARG A 176   -16.248   1.967 -21.167  1.00 14.64      A
ATOM   1365  CG  ARG A 176   -15.987   2.385 -19.734  1.00 15.67      A
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Figure 1 (continued 14)

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ATOM   1366  CD   ARG A 176    -15.877    1.156  -18.816  1.00  15.21       A
ATOM   1367  NE   ARG A 176    -15.566    1.544  -17.439  1.00  14.17       A
ATOM   1368  CZ   ARG A 176    -14.353    1.799  -16.937  1.00  16.17       A
ATOM   1369  NH1  ARG A 176    -13.264    1.720  -17.703  1.00  14.70       A
ATOM   1370  NH2  ARG A 176    -14.223    2.102  -15.644  1.00  16.59       A
ATOM   1371  C    ARG A 176    -18.026    0.146  -21.304  1.00  12.49       A
ATOM   1372  O    ARG A 176    -18.629   -0.217  -20.280  1.00  13.08       A
ATOM   1373  N    LEU A 177    -17.628   -0.684  -22.262  1.00  11.81       A
ATOM   1374  CA   LEU A 177    -17.922   -2.105  -22.203  1.00  10.41       A
ATOM   1375  CB   LEU A 177    -19.100   -2.440  -23.151  1.00  11.88       A
ATOM   1376  CG   LEU A 177    -19.466   -3.935  -23.318  1.00  10.26       A
ATOM   1377  CD1  LEU A 177    -20.967   -4.089  -23.579  1.00  13.42       A
ATOM   1378  CD2  LEU A 177    -18.693   -4.547  -24.453  1.00  12.11       A
ATOM   1379  C    LEU A 177    -16.685   -2.882  -22.630  1.00  11.58       A
ATOM   1380  O    LEU A 177    -15.896   -2.415  -23.455  1.00  12.23       A
ATOM   1381  N    ALA A 178    -16.524   -4.055  -22.029  1.00  10.67       A
ATOM   1382  CA   ALA A 178    -15.417   -4.939  -22.349  1.00  11.62       A
ATOM   1383  CB   ALA A 178    -14.417   -5.005  -21.178  1.00  11.64       A
ATOM   1384  C    ALA A 178    -15.972   -6.330  -22.617  1.00  12.71       A
ATOM   1385  O    ALA A 178    -16.842   -6.774  -21.876  1.00  12.95       A
ATOM   1386  N    VAL A 179    -15.510   -7.003  -23.678  1.00  12.86       A
ATOM   1387  CA   VAL A 179    -15.960   -8.374  -23.931  1.00  11.78       A
ATOM   1388  CB   VAL A 179    -17.058   -8.434  -25.021  1.00  13.43       A
ATOM   1389  CG1  VAL A 179    -16.623   -7.680  -26.291  1.00  13.32       A
ATOM   1390  CG2  VAL A 179    -17.401   -9.905  -25.341  1.00  13.70       A
ATOM   1391  C    VAL A 179    -14.771   -9.221  -24.330  1.00  12.02       A
ATOM   1392  O    VAL A 179    -13.897   -8.750  -25.047  1.00  13.44       A
ATOM   1393  N    CYS A 180    -14.736  -10.463  -23.853  1.00  11.67       A
ATOM   1394  CA   CYS A 180    -13.611  -11.330  -24.205  1.00  12.63       A
ATOM   1395  CB   CYS A 180    -12.567  -11.260  -23.107  1.00  12.65       A
ATOM   1396  SG   CYS A 180    -11.064  -12.233  -23.457  1.00  16.29       A
ATOM   1397  C    CYS A 180    -14.123  -12.752  -24.329  1.00  14.48       A
ATOM   1398  O    CYS A 180    -14.900  -13.187  -23.487  1.00  14.59       A
ATOM   1399  N    SER A 181    -13.722  -13.467  -25.379  1.00  14.95       A
ATOM   1400  CA   SER A 181    -14.178  -14.859  -25.516  1.00  17.59       A
ATOM   1401  CB   SER A 181    -15.229  -15.019  -26.640  1.00  20.93       A
ATOM   1402  OG   SER A 181    -14.687  -14.808  -27.912  1.00  26.78       A
ATOM   1403  C    SER A 181    -12.970  -15.726  -25.794  1.00  17.42       A
ATOM   1404  O    SER A 181    -12.009  -15.274  -26.428  1.00  18.86       A
ATOM   1405  N    MET A 182    -13.020  -16.953  -25.305  1.00  16.52       A
ATOM   1406  CA   MET A 182    -11.929  -17.925  -25.453  1.00  17.26       A
ATOM   1407  CB   MET A 182    -11.075  -17.953  -24.177  1.00  20.28       A
ATOM   1408  CG   MET A 182    -10.358  -16.670  -23.853  1.00  22.98       A
ATOM   1409  SD   MET A 182     -8.999  -16.391  -24.945  1.00  26.97       A
ATOM   1410  CE   MET A 182     -7.746  -17.563  -24.206  1.00  26.51       A
ATOM   1411  C    MET A 182    -12.489  -19.310  -25.681  1.00  18.28       A
ATOM   1412  O    MET A 182    -13.421  -19.734  -25.022  1.00  17.56       A
ATOM   1413  N    PRO A 183    -11.906  -20.056  -26.629  1.00  19.27       A
ATOM   1414  CD   PRO A 183    -10.796  -19.620  -27.496  1.00  19.63       A
ATOM   1415  CA   PRO A 183    -12.345  -21.411  -26.955  1.00  20.53       A
ATOM   1416  CB   PRO A 183    -11.645  -21.677  -28.300  1.00  21.37       A
ATOM   1417  CG   PRO A 183    -10.352  -20.944  -28.145  1.00  21.39       A
ATOM   1418  C    PRO A 183    -11.899  -22.371  -25.856  1.00  21.32       A
ATOM   1419  O    PRO A 183    -10.802  -22.220  -25.296  1.00  22.60       A
ATOM   1420  N    ILE A 184    -12.748  -23.327  -25.517  1.00  21.08       A
ATOM   1421  CA   ILE A 184    -12.345  -24.269  -24.494  1.00  23.29       A
ATOM   1422  CB   ILE A 184    -13.118  -24.019  -23.185  1.00  22.91       A
ATOM   1423  CG2  ILE A 184    -12.720  -22.669  -22.621  1.00  23.87       A
ATOM   1424  CG1  ILE A 184    -14.624  -24.034  -23.439  1.00  24.45       A
ATOM   1425  CD1  ILE A 184    -15.454  -23.874  -22.154  1.00  28.40       A
ATOM   1426  C    ILE A 184    -12.427  -25.733  -24.928  1.00  23.80       A
ATOM   1427  O    ILE A 184    -12.332  -26.637  -24.103  1.00  24.50       A
ATOM   1428  N    GLY A 185    -12.597  -25.964  -26.225  1.00  26.05       A
ATOM   1429  CA   GLY A 185    -12.600  -27.329  -26.740  1.00  25.71       A
ATOM   1430  C    GLY A 185    -13.698  -28.288  -26.348  1.00  27.58       A
ATOM   1431  O    GLY A 185    -13.512  -29.516  -26.410  1.00  27.68       A
ATOM   1432  N    GLN A 186    -14.844  -27.738  -25.968  1.00  26.74       A
ATOM   1433  CA   GLN A 186    -16.006  -28.518  -25.573  1.00  27.53       A
ATOM   1434  CB   GLN A 186    -16.150  -28.518  -24.048  1.00  28.12       A
ATOM   1435  CG   GLN A 186    -14.938  -29.039  -23.330  1.00  28.26       A
ATOM   1436  CD   GLN A 186    -14.790  -28.436  -21.949  1.00  29.33       A
ATOM   1437  OE1  GLN A 186    -15.532  -28.775  -21.025  1.00  28.19       A
ATOM   1438  NE2  GLN A 186    -13.834  -27.525  -21.808  1.00  29.64       A
ATOM   1439  C    GLN A 186    -17.217  -27.837  -26.192  1.00  27.94       A
ATOM   1440  O    GLN A 186    -17.297  -26.613  -26.227  1.00  27.59       A
ATOM   1441  N    SER A 187    -18.156  -28.632  -26.687  1.00  29.04       A
ATOM   1442  CA   SER A 187    -19.368  -28.105  -27.290  1.00  28.26       A
ATOM   1443  CB   SER A 187    -19.987  -29.173  -28.202  1.00  30.89       A
ATOM   1444  OG   SER A 187    -21.163  -28.684  -28.826  1.00  35.18       A
ATOM   1445  C    SER A 187    -20.294  -27.770  -26.120  1.00  27.81       A
ATOM   1446  O    SER A 187    -20.650  -28.652  -25.339  1.00  28.41       A
ATOM   1447  N    LEU A 188    -20.681  -26.502  -26.000  1.00  25.54       A
ATOM   1448  CA   LEU A 188    -21.504  -26.055  -24.875  1.00  23.98       A
ATOM   1449  CB   LEU A 188    -20.785  -24.911  -24.136  1.00  23.58       A
ATOM   1450  CG   LEU A 188    -19.296  -25.012  -23.823  1.00  23.00       A
ATOM   1451  CD1  LEU A 188    -18.653  -23.602  -23.655  1.00  22.33       A
ATOM   1452  CD2  LEU A 188    -19.138  -25.849  -22.567  1.00  23.44       A
ATOM   1453  C    LEU A 188    -22.883  -25.548  -25.235  1.00  24.43       A
ATOM   1454  O    LEU A 188    -23.105  -25.040  -26.341  1.00  23.24       A
ATOM   1455  N    PRO A 189    -23.843  -25.694  -24.308  1.00  24.44       A
ATOM   1456  CD   PRO A 189    -23.775  -26.479  -23.057  1.00  26.09       A
ATOM   1457  CA   PRO A 189    -25.204  -25.207  -24.547  1.00  24.88       A
ATOM   1458  CB   PRO A 189    -26.014  -25.858  -23.420  1.00  26.37       A
ATOM   1459  CG   PRO A 189    -25.007  -25.986  -22.303  1.00  25.65       A
ATOM   1460  C    PRO A 189    -25.111  -23.687  -24.375  1.00  25.47       A
ATOM   1461  O    PRO A 189    -24.212  -23.195  -23.668  1.00  24.66       A
ATOM   1462  N    SER A 190    -26.019  -22.948  -25.005  1.00  25.63       A
ATOM   1463  CA   SER A 190    -26.009  -21.492  -24.887  1.00  25.88       A
ATOM   1464  CB   SER A 190    -26.878  -20.866  -25.960  1.00  26.21       A
ATOM   1465  OG   SER A 190    -26.413  -21.232  -27.230  1.00  31.10       A
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Figure 1 (continued 15)

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ATOM   1466  C    SER A 190    -26.546 -21.121 -23.537  1.00 25.83       A
ATOM   1467  O    SER A 190    -27.690 -21.444 -23.194  1.00 26.64       A
ATOM   1468  N    HIS A 191    -25.741 -20.414 -22.757  1.00 24.59       A
ATOM   1469  CA   HIS A 191    -26.179 -20.046 -21.424  1.00 23.84       A
ATOM   1470  CB   HIS A 191    -25.761 -21.123 -20.433  1.00 28.01       A
ATOM   1471  CG   HIS A 191    -26.680 -21.250 -19.267  1.00 33.05       A
ATOM   1472  CD2  HIS A 191    -26.528 -20.901 -17.966  1.00 33.83       A
ATOM   1473  ND1  HIS A 191    -27.956 -21.759 -19.383  1.00 34.03       A
ATOM   1474  CE1  HIS A 191    -28.552 -21.716 -18.202  1.00 34.58       A
ATOM   1475  NE2  HIS A 191    -27.708 -21.200 -17.326  1.00 35.13       A
ATOM   1476  C    HIS A 191    -25.529 -18.727 -21.035  1.00 21.91       A
ATOM   1477  O    HIS A 191    -24.404 -18.450 -21.444  1.00 19.14       A
ATOM   1478  N    SER A 192    -26.236 -17.937 -20.238  1.00 18.95       A
ATOM   1479  CA   SER A 192    -25.741 -16.633 -19.821  1.00 19.59       A
ATOM   1480  CB   SER A 192    -26.394 -15.574 -20.743  1.00 22.50       A
ATOM   1481  OG   SER A 192    -26.222 -14.238 -20.342  1.00 27.62       A
ATOM   1482  C    SER A 192    -26.135 -16.407 -18.360  1.00 19.05       A
ATOM   1483  O    SER A 192    -27.304 -16.593 -18.004  1.00 21.16       A
ATOM   1484  N    VAL A 193    -25.165 -16.043 -17.524  1.00 16.50       A
ATOM   1485  CA   VAL A 193    -25.407 -15.734 -16.095  1.00 14.76       A
ATOM   1486  CB   VAL A 193    -25.093 -16.937 -15.138  1.00 13.63       A
ATOM   1487  CG1  VAL A 193    -25.999 -18.109 -15.494  1.00 17.20       A
ATOM   1488  CG2  VAL A 193    -23.620 -17.348 -15.216  1.00 15.41       A
ATOM   1489  C    VAL A 193    -24.538 -14.560 -15.664  1.00 14.41       A
ATOM   1490  O    VAL A 193    -23.516 -14.254 -16.291  1.00 12.96       A
ATOM   1491  N    ILE A 194    -24.968 -13.886 -14.607  1.00 12.61       A
ATOM   1492  CA   ILE A 194    -24.252 -12.716 -14.085  1.00 11.47       A
ATOM   1493  CB   ILE A 194    -25.213 -11.508 -13.867  1.00 12.39       A
ATOM   1494  CG2  ILE A 194    -24.396 -10.299 -13.430  1.00 12.88       A
ATOM   1495  CG1  ILE A 194    -25.983 -11.198 -15.146  1.00 14.24       A
ATOM   1496  CD1  ILE A 194    -27.031 -10.095 -14.967  1.00 17.17       A
ATOM   1497  C    ILE A 194    -23.660 -13.080 -12.736  1.00 13.07       A
ATOM   1498  O    ILE A 194    -24.376 -13.466 -11.803  1.00 13.64       A
ATOM   1499  N    VAL A 195    -22.336 -13.004 -12.632  1.00 12.90       A
ATOM   1500  CA   VAL A 195    -21.654 -13.314 -11.385  1.00 14.01       A
ATOM   1501  CB   VAL A 195    -20.301 -14.008 -11.696  1.00 15.92       A
ATOM   1502  CG1  VAL A 195    -19.560 -14.344 -10.413  1.00 14.56       A
ATOM   1503  CG2  VAL A 195    -20.545 -15.287 -12.497  1.00 13.57       A
ATOM   1504  C    VAL A 195    -21.424 -11.989 -10.641  1.00 13.97       A
ATOM   1505  O    VAL A 195    -20.949 -11.041 -11.214  1.00 14.63       A
ATOM   1506  N    PRO A 196    -21.783 -11.915  -9.351  1.00 15.51       A
ATOM   1507  CD   PRO A 196    -22.324 -12.986  -8.492  1.00 16.27       A
ATOM   1508  CA   PRO A 196    -21.573 -10.657  -8.622  1.00 16.07       A
ATOM   1509  CB   PRO A 196    -22.178 -10.929  -7.241  1.00 17.85       A
ATOM   1510  CG   PRO A 196    -22.132 -12.418  -7.098  1.00 18.14       A
ATOM   1511  C    PRO A 196    -20.114 -10.220  -8.553  1.00 16.89       A
ATOM   1512  O    PRO A 196    -19.202 -11.051  -8.543  1.00 15.71       A
ATOM   1513  N    ARG A 197    -19.868  -8.916  -8.473  1.00 17.07       A
ATOM   1514  CA   ARG A 197    -18.470  -8.494  -8.456  1.00 19.18       A
ATOM   1515  CB   ARG A 197    -18.351  -6.965  -8.477  1.00 23.00       A
ATOM   1516  CG   ARG A 197    -19.035  -6.236  -7.375  1.00 26.04       A
ATOM   1517  CD   ARG A 197    -18.680  -4.725  -7.481  1.00 28.79       A
ATOM   1518  NE   ARG A 197    -17.228  -4.495  -7.441  1.00 32.92       A
ATOM   1519  CZ   ARG A 197    -16.496  -4.048  -8.463  1.00 34.73       A
ATOM   1520  NH1  ARG A 197    -17.059  -3.761  -9.628  1.00 36.57       A
ATOM   1521  NH2  ARG A 197    -15.185  -3.905  -8.329  1.00 37.08       A
ATOM   1522  C    ARG A 197    -17.590  -9.107  -7.376  1.00 18.61       A
ATOM   1523  O    ARG A 197    -16.447  -9.437  -7.645  1.00 19.10       A
ATOM   1524  N    LYS A 198    -18.106  -9.310  -6.165  1.00 19.11       A
ATOM   1525  CA   LYS A 198    -17.295  -9.924  -5.130  1.00 21.70       A
ATOM   1526  CB   LYS A 198    -18.032  -9.861  -3.790  1.00 24.75       A
ATOM   1527  CG   LYS A 198    -17.243 -10.408  -2.616  1.00 30.79       A
ATOM   1528  CD   LYS A 198    -17.904  -9.948  -1.300  1.00 32.84       A
ATOM   1529  CE   LYS A 198    -17.265 -10.606  -0.086  1.00 35.71       A
ATOM   1530  NZ   LYS A 198    -17.913 -10.169   1.206  1.00 35.61       A
ATOM   1531  C    LYS A 198    -16.943 -11.377  -5.492  1.00 20.89       A
ATOM   1532  O    LYS A 198    -15.864 -11.885  -5.152  1.00 21.60       A
ATOM   1533  N    GLY A 199    -17.844 -12.052  -6.205  1.00 19.66       A
ATOM   1534  CA   GLY A 199    -17.583 -13.421  -6.613  1.00 18.99       A
ATOM   1535  C    GLY A 199    -16.488 -13.483  -7.678  1.00 17.60       A
ATOM   1536  O    GLY A 199    -15.678 -14.406  -7.751  1.00 18.00       A
ATOM   1537  N    VAL A 200    -16.492 -12.486  -8.553  1.00 18.22       A
ATOM   1538  CA   VAL A 200    -15.498 -12.422  -9.610  1.00 16.49       A
ATOM   1539  CB   VAL A 200    -15.780 -11.199 -10.534  1.00 15.63       A
ATOM   1540  CG1  VAL A 200    -14.604 -11.013 -11.522  1.00 16.76       A
ATOM   1541  CG2  VAL A 200    -17.104 -11.417 -11.287  1.00 17.52       A
ATOM   1542  C    VAL A 200    -14.097 -12.289  -8.978  1.00 18.83       A
ATOM   1543  O    VAL A 200    -13.138 -12.928  -9.425  1.00 19.59       A
ATOM   1544  N    ILE A 201    -14.002 -11.465  -7.937  1.00 21.69       A
ATOM   1545  CA   ILE A 201    -12.735 -11.240  -7.220  1.00 24.32       A
ATOM   1546  CB   ILE A 201    -12.897 -10.278  -6.026  1.00 26.86       A
ATOM   1547  CG2  ILE A 201    -11.547 -10.101  -5.327  1.00 28.23       A
ATOM   1548  CG1  ILE A 201    -13.504  -8.954  -6.471  1.00 28.44       A
ATOM   1549  CD1  ILE A 201    -13.047  -8.463  -7.799  1.00 29.79       A
ATOM   1550  C    ILE A 201    -12.227 -12.531  -6.619  1.00 24.50       A
ATOM   1551  O    ILE A 201    -11.042 -12.872  -6.721  1.00 24.04       A
ATOM   1552  N    GLU A 202    -13.141 -13.234  -5.971  1.00 26.55       A
ATOM   1553  CA   GLU A 202    -12.854 -14.491  -5.319  1.00 29.06       A
ATOM   1554  CB   GLU A 202    -14.113 -14.972  -4.574  1.00 32.98       A
ATOM   1555  CG   GLU A 202    -13.831 -15.705  -3.291  1.00 36.13       A
ATOM   1556  CD   GLU A 202    -12.688 -15.076  -2.521  1.00 38.29       A
ATOM   1557  OE1  GLU A 202    -12.804 -13.893  -2.097  1.00 38.50       A
ATOM   1558  OE2  GLU A 202    -11.665 -15.777  -2.356  1.00 39.57       A
ATOM   1559  C    GLU A 202    -12.405 -15.522  -6.346  1.00 29.59       A
ATOM   1560  O    GLU A 202    -11.447 -16.263  -6.117  1.00 29.66       A
ATOM   1561  N    LEU A 203    -13.080 -15.573  -7.490  1.00 28.27       A
ATOM   1562  CA   LEU A 203    -12.706 -16.519  -8.529  1.00 28.89       A
ATOM   1563  CB   LEU A 203    -13.595 -16.352  -9.761  1.00 31.21       A
ATOM   1564  CG   LEU A 203    -14.700 -17.368 -10.014  1.00 31.78       A
ATOM   1565  CD1  LEU A 203    -15.388 -17.044 -11.313  1.00 30.83       A
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Figure 1 (continued 16)

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ATOM   1566  CD2 LEU A 203    -14.090 -18.768 -10.061  1.00 32.03      A
ATOM   1567  C   LEU A 203    -11.260 -16.256  -8.929  1.00 29.61      A
ATOM   1568  O   LEU A 203    -10.459 -17.171  -9.072  1.00 27.41      A
ATOM   1569  N   MET A 204    -10.951 -14.984  -9.134  1.00 28.89      A
ATOM   1570  CA  MET A 204     -9.615 -14.578  -9.514  1.00 31.07      A
ATOM   1571  CB  MET A 204     -9.589 -13.048  -9.635  1.00 32.20      A
ATOM   1572  CG  MET A 204     -8.538 -12.491 -10.565  1.00 36.14      A
ATOM   1573  SD  MET A 204     -8.637 -13.238 -12.199  1.00 37.25      A
ATOM   1574  CE  MET A 204     -7.159 -14.209 -12.153  1.00 38.24      A
ATOM   1575  C   MET A 204     -8.599 -15.060  -8.463  1.00 32.05      A
ATOM   1576  O   MET A 204     -7.545 -15.592  -8.813  1.00 31.41      A
ATOM   1577  N   ARG A 205     -8.936 -14.905  -7.182  1.00 33.59      A
ATOM   1578  CA  ARG A 205     -8.040 -15.287  -6.071  1.00 36.58      A
ATOM   1579  CB  ARG A 205     -8.659 -14.940  -4.707  1.00 38.43      A
ATOM   1580  CG  ARG A 205     -9.093 -13.505  -4.521  1.00 42.16      A
ATOM   1581  CD  ARG A 205     -7.928 -12.549  -4.307  1.00 45.61      A
ATOM   1582  NE  ARG A 205     -8.409 -11.165  -4.316  1.00 47.97      A
ATOM   1583  CZ  ARG A 205     -7.674 -10.093  -4.029  1.00 48.71      A
ATOM   1584  NH1 ARG A 205     -6.392 -10.219  -3.694  1.00 49.29      A
ATOM   1585  NH2 ARG A 205     -8.227  -8.886  -4.092  1.00 49.19      A
ATOM   1586  C   ARG A 205     -7.643 -16.752  -6.002  1.00 37.14      A
ATOM   1587  O   ARG A 205     -6.571 -17.088  -5.492  1.00 37.07      A
ATOM   1588  N   MET A 206     -8.496 -17.641  -6.482  1.00 37.50      A
ATOM   1589  CA  MET A 206     -8.162 -19.049  -6.380  1.00 39.03      A
ATOM   1590  CB  MET A 206     -9.435 -19.869  -6.144  1.00 39.34      A
ATOM   1591  CG  MET A 206    -10.340 -19.984  -7.341  1.00 39.33      A
ATOM   1592  SD  MET A 206    -11.995 -20.514  -6.838  1.00 39.83      A
ATOM   1593  CE  MET A 206    -11.592 -22.096  -5.995  1.00 37.83      A
ATOM   1594  C   MET A 206     -7.403 -19.572  -7.587  1.00 40.42      A
ATOM   1595  O   MET A 206     -7.071 -20.759  -7.657  1.00 39.42      A
ATOM   1596  N   LEU A 207     -7.117 -18.686  -8.534  1.00 41.79      A
ATOM   1597  CA  LEU A 207     -6.403 -19.081  -9.744  1.00 45.36      A
ATOM   1598  CB  LEU A 207     -6.972 -18.329 -10.955  1.00 45.10      A
ATOM   1599  CG  LEU A 207     -8.187 -18.866 -11.721  1.00 46.04      A
ATOM   1600  CD1 LEU A 207     -9.219 -19.475 -10.799  1.00 45.64      A
ATOM   1601  CD2 LEU A 207     -8.791 -17.719 -12.517  1.00 46.42      A
ATOM   1602  C   LEU A 207     -4.903 -18.814  -9.629  1.00 47.44      A
ATOM   1603  O   LEU A 207     -4.487 -17.670  -9.432  1.00 48.80      A
ATOM   1604  N   ASP A 208     -4.103 -19.869  -9.761  1.00 49.36      A
ATOM   1605  CA  ASP A 208     -2.648 -19.759  -9.681  1.00 51.16      A
ATOM   1606  CB  ASP A 208     -2.126 -20.579  -8.504  1.00 52.20      A
ATOM   1607  CG  ASP A 208     -2.697 -20.119  -7.180  1.00 54.01      A
ATOM   1608  OD1 ASP A 208     -2.638 -18.896  -6.906  1.00 54.78      A
ATOM   1609  OD2 ASP A 208     -3.198 -20.978  -6.412  1.00 53.95      A
ATOM   1610  C   ASP A 208     -1.954 -20.216 -10.967  1.00 51.89      A
ATOM   1611  O   ASP A 208     -0.786 -20.611 -10.950  1.00 52.13      A
ATOM   1612  N   GLY A 209     -2.689 -20.168 -12.076  1.00 52.31      A
ATOM   1613  CA  GLY A 209     -2.144 -20.552 -13.366  1.00 52.06      A
ATOM   1614  C   GLY A 209     -1.567 -21.948 -13.502  1.00 52.17      A
ATOM   1615  O   GLY A 209     -0.961 -22.254 -14.533  1.00 52.89      A
ATOM   1616  N   GLY A 210     -1.737 -22.795 -12.488  1.00 51.34      A
ATOM   1617  CA  GLY A 210     -1.215 -24.152 -12.566  1.00 50.65      A
ATOM   1618  C   GLY A 210     -1.779 -24.891 -13.769  1.00 49.99      A
ATOM   1619  O   GLY A 210     -2.751 -24.435 -14.367  1.00 49.83      A
ATOM   1620  N   ASP A 211     -1.180 -26.023 -14.135  1.00 49.29      A
ATOM   1621  CA  ASP A 211     -1.656 -26.803 -15.283  1.00 48.42      A
ATOM   1622  CB  ASP A 211     -0.602 -27.833 -15.701  1.00 49.93      A
ATOM   1623  CG  ASP A 211      0.655 -27.184 -16.261  1.00 51.04      A
ATOM   1624  OD1 ASP A 211      0.568 -26.549 -17.334  1.00 52.21      A
ATOM   1625  OD2 ASP A 211      1.725 -27.303 -15.627  1.00 52.08      A
ATOM   1626  C   ASP A 211     -2.953 -27.508 -14.910  1.00 47.33      A
ATOM   1627  O   ASP A 211     -3.642 -28.077 -15.759  1.00 47.11      A
ATOM   1628  N   ASN A 212     -3.247 -27.442 -13.616  1.00 45.10      A
ATOM   1629  CA  ASN A 212     -4.425 -28.013 -12.974  1.00 43.75      A
ATOM   1630  CB  ASN A 212     -4.245 -27.801 -11.463  1.00 44.05      A
ATOM   1631  CG  ASN A 212     -5.009 -28.795 -10.619  1.00 45.06      A
ATOM   1632  OD1 ASN A 212     -4.957 -28.731  -9.387  1.00 44.49      A
ATOM   1633  ND2 ASN A 212     -5.715 -29.722 -11.263  1.00 45.44      A
ATOM   1634  C   ASN A 212     -5.653 -27.237 -13.497  1.00 41.13      A
ATOM   1635  O   ASN A 212     -5.779 -26.045 -13.252  1.00 42.29      A
ATOM   1636  N   PRO A 213     -6.573 -27.899 -14.221  1.00 38.67      A
ATOM   1637  CD  PRO A 213     -6.625 -29.292 -14.698  1.00 38.16      A
ATOM   1638  CA  PRO A 213     -7.731 -27.143 -14.716  1.00 35.46      A
ATOM   1639  CB  PRO A 213     -8.264 -28.026 -15.829  1.00 36.69      A
ATOM   1640  CG  PRO A 213     -8.037 -29.389 -15.267  1.00 38.80      A
ATOM   1641  C   PRO A 213     -8.806 -26.834 -13.686  1.00 32.37      A
ATOM   1642  O   PRO A 213     -8.897 -27.468 -12.635  1.00 32.62      A
ATOM   1643  N   LEU A 214     -9.622 -25.840 -14.013  1.00 29.01      A
ATOM   1644  CA  LEU A 214    -10.734 -25.415 -13.172  1.00 26.42      A
ATOM   1645  CB  LEU A 214    -10.934 -23.896 -13.338  1.00 27.73      A
ATOM   1646  CG  LEU A 214    -12.055 -23.149 -12.622  1.00 29.04      A
ATOM   1647  CD1 LEU A 214    -11.718 -23.086 -11.170  1.00 31.24      A
ATOM   1648  CD2 LEU A 214    -12.194 -21.719 -13.164  1.00 29.62      A
ATOM   1649  C   LEU A 214    -11.979 -26.163 -13.663  1.00 24.15      A
ATOM   1650  O   LEU A 214    -12.179 -26.296 -14.867  1.00 23.32      A
ATOM   1651  N   ARG A 215    -12.803 -26.670 -12.751  1.00 20.02      A
ATOM   1652  CA  ARG A 215    -14.025 -27.355 -13.139  1.00 20.46      A
ATOM   1653  CB  ARG A 215    -14.132 -28.715 -12.415  1.00 25.18      A
ATOM   1654  CG  ARG A 215    -12.876 -29.577 -12.626  1.00 31.55      A
ATOM   1655  CD  ARG A 215    -13.031 -31.025 -12.142  1.00 37.20      A
ATOM   1656  NE  ARG A 215    -13.414 -31.946 -13.221  1.00 42.35      A
ATOM   1657  CZ  ARG A 215    -14.626 -32.003 -13.779  1.00 44.98      A
ATOM   1658  NH1 ARG A 215    -15.597 -31.192 -13.360  1.00 46.39      A
ATOM   1659  NH2 ARG A 215    -14.871 -32.862 -14.771  1.00 44.99      A
ATOM   1660  C   ARG A 215    -15.158 -26.422 -12.724  1.00 18.21      A
ATOM   1661  O   ARG A 215    -15.280 -26.064 -11.564  1.00 18.66      A
ATOM   1662  N   VAL A 216    -15.978 -26.026 -13.682  1.00 15.42      A
ATOM   1663  CA  VAL A 216    -17.061 -25.082 -13.410  1.00 15.50      A
ATOM   1664  CB  VAL A 216    -16.988 -23.890 -14.404  1.00 14.33      A
ATOM   1665  CG1 VAL A 216    -18.154 -22.945 -14.149  1.00 16.88      A
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Figure 1 (continued 17)

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ATOM   1666  CG2 VAL A 216     -15.661 -23.199 -14.269  1.00 16.10      A
ATOM   1667  C   VAL A 216     -18.420 -25.727 -13.568  1.00 15.31      A
ATOM   1668  O   VAL A 216     -18.641 -26.525 -14.488  1.00 18.21      A
ATOM   1669  N   GLN A 217     -19.347 -25.373 -12.680  1.00 15.12      A
ATOM   1670  CA  GLN A 217     -20.696 -25.879 -12.745  1.00 16.55      A
ATOM   1671  CB  GLN A 217     -21.001 -26.859 -11.607  1.00 17.03      A
ATOM   1672  CG  GLN A 217     -20.322 -28.182 -11.686  1.00 17.24      A
ATOM   1673  CD  GLN A 217     -20.607 -29.052 -10.445  1.00 19.83      A
ATOM   1674  OE1 GLN A 217     -20.179 -28.723  -9.334  1.00 24.23      A
ATOM   1675  NE2 GLN A 217     -21.341 -30.150 -10.636  1.00 22.05      A
ATOM   1676  C   GLN A 217     -21.590 -24.655 -12.596  1.00 16.13      A
ATOM   1677  O   GLN A 217     -21.412 -23.872 -11.675  1.00 16.81      A
ATOM   1678  N   ILE A 218     -22.543 -24.485 -13.510  1.00 16.16      A
ATOM   1679  CA  ILE A 218     -23.457 -23.338 -13.436  1.00 14.93      A
ATOM   1680  CB  ILE A 218     -23.312 -22.443 -14.721  1.00 17.67      A
ATOM   1681  CG2 ILE A 218     -24.342 -21.285 -14.709  1.00 19.90      A
ATOM   1682  CG1 ILE A 218     -21.885 -21.891 -14.797  1.00 18.86      A
ATOM   1683  CD1 ILE A 218     -21.559 -21.069 -16.069  1.00 20.21      A
ATOM   1684  C   ILE A 218     -24.895 -23.824 -13.317  1.00 16.21      A
ATOM   1685  O   ILE A 218     -25.327 -24.690 -14.080  1.00 17.78      A
ATOM   1686  N   GLY A 219     -25.622 -23.261 -12.357  1.00 16.39      A
ATOM   1687  CA  GLY A 219     -27.028 -23.573 -12.144  1.00 17.69      A
ATOM   1688  C   GLY A 219     -27.886 -22.361 -12.487  1.00 19.32      A
ATOM   1689  O   GLY A 219     -27.381 -21.370 -12.982  1.00 20.27      A
ATOM   1690  N   SER A 220     -29.188 -22.425 -12.243  1.00 20.22      A
ATOM   1691  CA  SER A 220     -30.033 -21.285 -12.570  1.00 21.44      A
ATOM   1692  CB  SER A 220     -31.498 -21.655 -12.408  1.00 22.40      A
ATOM   1693  OG  SER A 220     -31.780 -22.064 -11.071  1.00 25.42      A
ATOM   1694  C   SER A 220     -29.741 -20.079 -11.690  1.00 21.28      A
ATOM   1695  O   SER A 220     -29.925 -18.935 -12.113  1.00 20.79      A
ATOM   1696  N   ASN A 221     -29.283 -20.337 -10.470  1.00 19.85      A
ATOM   1697  CA  ASN A 221     -29.033 -19.257  -9.523  1.00 20.14      A
ATOM   1698  CB  ASN A 221     -30.174 -19.212  -8.498  1.00 23.10      A
ATOM   1699  CG  ASN A 221     -31.536 -18.962  -9.162  1.00 26.82      A
ATOM   1700  OD1 ASN A 221     -32.207 -19.897  -9.622  1.00 31.73      A
ATOM   1701  ND2 ASN A 221     -31.927 -17.700  -9.245  1.00 27.82      A
ATOM   1702  C   ASN A 221     -27.704 -19.312  -8.798  1.00 17.29      A
ATOM   1703  O   ASN A 221     -27.487 -18.567  -7.845  1.00 16.83      A
ATOM   1704  N   ASN A 222     -26.814 -20.188  -9.249  1.00 16.78      A
ATOM   1705  CA  ASN A 222     -25.523 -20.298  -8.582  1.00 15.72      A
ATOM   1706  CB  ASN A 222     -25.543 -21.424  -7.526  1.00 18.61      A
ATOM   1707  CG  ASN A 222     -26.571 -21.210  -6.432  1.00 20.68      A
ATOM   1708  OD1 ASN A 222     -27.756 -21.491  -6.615  1.00 22.08      A
ATOM   1709  ND2 ASN A 222     -26.125 -20.705  -5.297  1.00 23.78      A
ATOM   1710  C   ASN A 222     -24.439 -20.686  -9.564  1.00 13.83      A
ATOM   1711  O   ASN A 222     -24.736 -21.188 -10.637  1.00 14.52      A
ATOM   1712  N   ILE A 223     -23.170 -20.449  -9.191  1.00 12.97      A
ATOM   1713  CA  ILE A 223     -22.034 -20.910 -10.008  1.00 13.44      A
ATOM   1714  CB  ILE A 223     -21.357 -19.742 -10.831  1.00 12.76      A
ATOM   1715  CG2 ILE A 223     -20.893 -18.636  -9.884  1.00 13.49      A
ATOM   1716  CG1 ILE A 223     -20.166 -20.277 -11.648  1.00 13.07      A
ATOM   1717  CD1 ILE A 223     -19.880 -19.360 -12.824  1.00 15.33      A
ATOM   1718  C   ILE A 223     -21.027 -21.498  -8.989  1.00 13.40      A
ATOM   1719  O   ILE A 223     -20.880 -20.994  -7.866  1.00 13.37      A
ATOM   1720  N   ARG A 224     -20.373 -22.578  -9.388  1.00 12.68      A
ATOM   1721  CA  ARG A 224     -19.398 -23.229  -8.544  1.00 13.73      A
ATOM   1722  CB  ARG A 224     -19.948 -24.578  -8.058  1.00 16.50      A
ATOM   1723  CG  ARG A 224     -18.928 -25.397  -7.280  1.00 18.24      A
ATOM   1724  CD  ARG A 224     -19.612 -26.522  -6.521  1.00 21.35      A
ATOM   1725  NE  ARG A 224     -20.401 -25.966  -5.432  1.00 23.07      A
ATOM   1726  CZ  ARG A 224     -21.253 -26.655  -4.680  1.00 25.49      A
ATOM   1727  NH1 ARG A 224     -21.440 -27.954  -4.897  1.00 27.26      A
ATOM   1728  NH2 ARG A 224     -21.935 -36.039  -3.721  1.00 27.55      A
ATOM   1729  C   ARG A 224     -18.152 -23.471  -9.370  1.00 13.92      A
ATOM   1730  O   ARG A 224     -18.217 -23.780 -10.567  1.00 13.44      A
ATOM   1731  N   ALA A 225     -17.014 -23.302  -8.723  1.00 13.45      A
ATOM   1732  CA  ALA A 225     -15.738 -23.582  -9.362  1.00 15.31      A
ATOM   1733  CB  ALA A 225     -15.027 -22.310  -9.670  1.00 16.60      A
ATOM   1734  C   ALA A 225     -14.892 -24.435  -8.419  1.00 16.41    ) A
ATOM   1735  O   ALA A 225     -14.763 -24.128  -7.236  1.00 15.00      A
ATOM   1736  N   HIS A 226     -14.310 -25.501  -8.961  1.00 17.50      A
ATOM   1737  CA  HIS A 226     -13.467 -26.417  -8.187  1.00 19.53      A
ATOM   1738  CB  HIS A 226     -13.896 -27.882  -8.433  1.00 23.40      A
ATOM   1739  CG  HIS A 226     -15.351 -28.163  -8.216  1.00 24.26      A
ATOM   1740  CD2 HIS A 226     -16.444 -27.890  -8.972  1.00 26.04      A
ATOM   1741  ND1 HIS A 226     -15.813 -28.853  -7.111  1.00 26.55      A
ATOM   1742  CE1 HIS A 226     -17.123 -28.901  -7.194  1.00 26.31      A
ATOM   1743  NE2 HIS A 226     -17.532 -28.420  -8.314  1.00 27.11      A
ATOM   1744  C   HIS A 226     -12.027 -26.291  -8.703  1.00 22.32      A
ATOM   1745  O   HIS A 226     -11.794 -26.492  -9.899  1.00 21.45      A
ATOM   1746  N   VAL A 227     -11.077 -25.951  -7.832  1.00 22.02      A
ATOM   1747  CA  VAL A 227      -9.660 -25.869  -8.218  1.00 26.25      A
ATOM   1748  CB  VAL A 227      -9.119 -24.414  -8.243  1.00 28.90      A
ATOM   1749  CG1 VAL A 227      -7.857 -24.334  -9.076  1.00 30.53      A
ATOM   1750  CG2 VAL A 227     -10.153 -23.489  -8.788  1.00 31.33      A
ATOM   1751  C   VAL A 227      -8.913 -26.600  -7.121  1.00 26.06      A
ATOM   1752  O   VAL A 227      -8.965 -26.192  -5.963  1.00 25.67      A
ATOM   1753  N   GLY A 228      -8.197 -27.651  -7.480  1.00 25.91      A
ATOM   1754  CA  GLY A 228      -7.468 -28.410  -6.478  1.00 24.98      A
ATOM   1755  C   GLY A 228      -8.417 -28.855  -5.381  1.00 24.00      A
ATOM   1756  O   GLY A 228      -9.469 -29.398  -5.671  1.00 24.36      A
ATOM   1757  N   ASP A 229      -8.079 -28.516  -4.126  1.00 22.64      A
ATOM   1758  CA  ASP A 229      -8.978 -29.011  -3.059  1.00 22.40      A
ATOM   1759  CB  ASP A 229      -8.214 -29.766  -1.989  1.00 24.16      A
ATOM   1760  CG  ASP A 229      -7.531 -31.019  -2.540  1.00 26.13      A
ATOM   1761  OD1 ASP A 229      -8.128 -31.718  -3.399  1.00 27.09      A
ATOM   1762  OD2 ASP A 229      -6.395 -31.293  -2.106  1.00 28.22      A
ATOM   1763  C   ASP A 229      -9.760 -27.837  -2.470  1.00 21.77      A
ATOM   1764  O   ASP A 229     -10.066 -27.791  -1.262  1.00 23.00      A
ATOM   1765  N   PHE A 230     -10.049 -26.873  -3.334  1.00 20.12      A
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Figure 1 (continued 18)

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ATOM   1766  CA   PHE A 230    -10.841 -25.701  -2.949  1.00 20.28      A
ATOM   1767  CB   PHE A 230    -10.082 -24.407  -3.238  1.00 20.97      A
ATOM   1768  CG   PHE A 230     -8.878 -24.208  -2.391  1.00 25.22      A
ATOM   1769  CD1  PHE A 230     -8.991 -23.676  -1.118  1.00 26.34      A
ATOM   1770  CD2  PHE A 230     -7.621 -24.553  -2.865  1.00 27.57      A
ATOM   1771  CE1  PHE A 230     -7.854 -23.486  -0.322  1.00 26.07      A
ATOM   1772  CE2  PHE A 230     -6.474 -24.365  -2.071  1.00 28.73      A
ATOM   1773  CZ   PHE A 230     -6.607 -23.828  -0.800  1.00 25.38      A
ATOM   1774  C    PHE A 230    -12.113 -25.691  -3.786  1.00 19.64      A
ATOM   1775  O    PHE A 230    -12.101 -26.056  -4.975  1.00 18.35      A
ATOM   1776  N    ILE A 231    -13.221 -25.307  -3.156  1.00 16.55      A
ATOM   1777  CA   ILE A 231    -14.492 -25.232  -3.873  1.00 16.98      A
ATOM   1778  CB   ILE A 231    -15.467 -26.329  -3.471  1.00 16.59      A
ATOM   1779  CG2  ILE A 231    -16.784 -26.149  -4.274  1.00 16.05      A
ATOM   1780  CG1  ILE A 231    -14.856 -27.717  -3.733  1.00 18.23      A
ATOM   1781  CD1  ILE A 231    -15.848 -28.868  -3.521  1.00 21.86      A
ATOM   1782  C    ILE A 231    -15.136 -23.900  -3.555  1.00 17.85      A
ATOM   1783  O    ILE A 231    -15.429 -23.581  -2.379  1.00 18.50      A
ATOM   1784  N    PHE A 232    -15.326 -23.109  -4.609  1.00 15.87      A
ATOM   1785  CA   PHE A 232    -15.943 -21.804  -4.487  1.00 15.49      A
ATOM   1786  CB   PHE A 232    -15.150 -20.771  -5.281  1.00 15.94      A
ATOM   1787  CG   PHE A 232    -15.792 -19.429  -5.269  1.00 18.31      A
ATOM   1788  CD1  PHE A 232    -15.921 -18.748  -4.066  1.00 20.92      A
ATOM   1789  CD2  PHE A 232    -16.283 -18.871  -6.431  1.00 20.41      A
ATOM   1790  CE1  PHE A 232    -16.539 -17.502  -4.018  1.00 21.57      A
ATOM   1791  CE2  PHE A 232    -16.915 -17.599  -6.399  1.00 19.94      A
ATOM   1792  CZ   PHE A 232    -17.032 -16.929  -5.200  1.00 21.00      A
ATOM   1793  C    PHE A 232    -17.349 -21.836  -5.060  1.00 14.79      A
ATOM   1794  O    PHE A 232    -17.556 -22.351  -6.142  1.00 14.73      A
ATOM   1795  N    THR A 233    -18.317 -21.261  -4.337  1.00 13.80      A
ATOM   1796  CA   THR A 233    -19.683 -21.214  -4.858  1.00 14.57      A
ATOM   1797  CB   THR A 233    -20.616 -22.226  -4.151  1.00 16.94      A
ATOM   1798  OG1  THR A 233    -20.009 -23.517  -4.157  1.00 17.68      A
ATOM   1799  CG2  THR A 233    -21.972 -22.310  -4.883  1.00 17.95      A
ATOM   1800  C    THR A 233    -20.236 -19.822  -4.603  1.00 14.93      A
ATOM   1801  O    THR A 233    -20.018 -19.237  -3.544  1.00 16.82      A
ATOM   1802  N    SER A 234    -20.927 -19.274  -5.590  1.00 14.49      A
ATOM   1803  CA   SER A 234    -21.543 -17.968  -5.406  1.00 13.46      A
ATOM   1804  CB   SER A 234    -20.743 -16.883  -6.136  1.00 13.74      A
ATOM   1805  OG   SER A 234    -21.424 -15.612  -6.057  1.00 15.56      A
ATOM   1806  C    SER A 234    -22.952 -17.945  -5.976  1.00 13.72      A
ATOM   1807  O    SER A 234    -23.272 -18.673  -6.914  1.00 14.31      A
ATOM   1808  N    LYS A 235    -23.796 -17.096  -5.384  1.00 14.72      A
ATOM   1809  CA   LYS A 235    -25.140 -16.882  -5.941  1.00 15.52      A
ATOM   1810  CB   LYS A 235    -26.017 -16.089  -4.965  1.00 18.32      A
ATOM   1811  CG   LYS A 235    -26.346 -16.843  -3.692  1.00 22.03      A
ATOM   1812  CD   LYS A 235    -27.446 -16.147  -2.881  1.00 26.96      A
ATOM   1813  CE   LYS A 235    -28.805 -16.273  -3.561  1.00 31.30      A
ATOM   1814  NZ   LYS A 235    -29.279 -17.699  -3.762  1.00 34.33      A
ATOM   1815  C    LYS A 235    -24.904 -16.023  -7.181  1.00 13.85      A
ATOM   1816  O    LYS A 235    -23.843 -15.357  -7.310  1.00 14.11      A
ATOM   1817  N    LEU A 236    -25.865 -16.060  -8.109  1.00 14.19      A
ATOM   1818  CA   LEU A 236    -25.790 -15.236  -9.322  1.00 14.29      A
ATOM   1819  CB   LEU A 236    -26.307 -16.007 -10.538  1.00 14.06      A
ATOM   1820  CG   LEU A 236    -25.517 -17.278 -10.914  1.00 13.43      A
ATOM   1821  CD1  LEU A 236    -26.211 -18.059 -12.011  1.00 15.03      A
ATOM   1822  CD2  LEU A 236    -24.085 -16.907 -11.375  1.00 13.57      A
ATOM   1823  C    LEU A 236    -26.661 -14.004  -9.095  1.00 15.56      A
ATOM   1824  O    LEU A 236    -27.429 -13.931  -8.119  1.00 18.35      A
ATOM   1825  N    VAL A 237    -26.555 -13.052  -9.998  1.00 14.01      A
ATOM   1826  CA   VAL A 237    -27.324 -11.803  -9.903  1.00 17.40      A
ATOM   1827  CB   VAL A 237    -26.462 -10.592 -10.324  1.00 16.42      A
ATOM   1828  CG1  VAL A 237    -27.275  -9.292 -10.179  1.00 18.55      A
ATOM   1829  CG2  VAL A 237    -25.205 -10.504  -9.471  1.00 17.94      A
ATOM   1830  C    VAL A 237    -28.516 -11.863 -10.844  1.00 19.10      A
ATOM   1831  O    VAL A 237    -28.394 -12.262 -12.003  1.00 19.48      A
ATOM   1832  N    ASP A 238    -29.683 -11.441 -10.368  1.00 23.53      A
ATOM   1833  CA   ASP A 238    -30.842 -11.424 -11.253  1.00 27.58      A
ATOM   1834  CB   ASP A 238    -32.129 -11.384 -10.441  1.00 31.74      A
ATOM   1835  CG   ASP A 238    -33.093 -12.485 -10.849  1.00 36.33      A
ATOM   1836  OD1  ASP A 238    -33.506 -12.522 -12.038  1.00 38.03      A
ATOM   1837  OD2  ASP A 238    -33.429 -13.318  -9.979  1.00 39.43      A
ATOM   1838  C    ASP A 238    -30.788 -10.205 -12.193  1.00 27.85      A
ATOM   1839  O    ASP A 238    -30.073  -9.224 -11.951  1.00 27.68      A
ATOM   1840  N    GLY A 239    -31.516 -10.272 -13.288  1.00 27.65      A
ATOM   1841  CA   GLY A 239    -31.524  -9.143 -14.185  1.00 27.62      A
ATOM   1842  C    GLY A 239    -31.152  -9.550 -15.580  1.00 28.08      A
ATOM   1843  O    GLY A 239    -30.584 -10.616 -15.790  1.00 28.81      A
ATOM   1844  N    ARG A 240    -31.491  -8.683 -16.521  1.00 29.63      A
ATOM   1845  CA   ARG A 240    -31.208  -8.878 -17.932  1.00 30.14      A
ATOM   1846  CB   ARG A 240    -32.392  -8.389 -18.771  1.00 33.69      A
ATOM   1847  CG   ARG A 240    -32.239  -8.574 -20.279  1.00 38.96      A
ATOM   1848  CD   ARG A 240    -32.122 -10.052 -20.651  1.00 43.41      A
ATOM   1849  NE   ARG A 240    -32.302 -10.267 -22.087  1.00 46.82      A
ATOM   1850  CZ   ARG A 240    -32.389 -11.460 -22.669  1.00 48.33      A
ATOM   1851  NH1  ARG A 240    -32.313 -12.570 -21.944  1.00 49.90      A
ATOM   1852  NH2  ARG A 240    -32.553 -11.543 -23.985  1.00 49.72      A
ATOM   1853  C    ARG A 240    -29.980  -8.040 -18.242  1.00 28.28      A
ATOM   1854  O    ARG A 240    -30.031  -6.814 -18.260  1.00 26.65      A
ATOM   1855  N    PHE A 241    -28.872  -8.718 -18.502  1.00 25.31      A
ATOM   1856  CA   PHE A 241    -27.633  -8.025 -18.822  1.00 23.21      A
ATOM   1857  CB   PHE A 241    -26.463  -9.006 -18.705  1.00 20.31      A
ATOM   1858  CG   PHE A 241    -25.146  -8.345 -18.481  1.00 17.38      A
ATOM   1859  CD1  PHE A 241    -24.780  -7.948 -17.206  1.00 15.49      A
ATOM   1860  CD2  PHE A 241    -24.297  -8.068 -19.549  1.00 17.91      A
ATOM   1861  CE1  PHE A 241    -23.586  -7.276 -16.980  1.00 15.90      A
ATOM   1862  CE2  PHE A 241    -23.102  -7.391 -19.330  1.00 14.47      A
ATOM   1863  CZ   PHE A 241    -22.747  -6.997 -18.051  1.00 15.32      A
ATOM   1864  C    PHE A 241    -27.711  -7.517 -20.271  1.00 22.81      A
ATOM   1865  O    PHE A 241    -28.322  -8.155 -21.137  1.00 24.71      A
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Figure 1 (continued 19)

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ATOM   1866  N    PRO A 242     -27.092   -6.365  -20.556  1.00 21.66           A
ATOM   1867  CD   PRO A 242     -26.466   -5.383  -19.664  1.00 20.82           A
ATOM   1868  CA   PRO A 242     -27.147   -5.870  -21.936  1.00 22.07           A
ATOM   1869  CB   PRO A 242     -26.503   -4.489  -21.849  1.00 23.09           A
ATOM   1870  CG   PRO A 242     -25.687   -4.543  -20.635  1.00 23.90           A
ATOM   1871  C    PRO A 242     -26.435   -6.788  -22.922  1.00 21.43           A
ATOM   1872  O    PRO A 242     -25.517   -7.513  -22.559  1.00 21.56           A
ATOM   1873  N    ASP A 243     -26.862   -6.730  -24.168  1.00 22.31           A
ATOM   1874  CA   ASP A 243     -26.325   -7.544  -25.235  1.00 22.61           A
ATOM   1875  CB   ASP A 243     -27.447   -7.789  -26.241  1.00 24.30           A
ATOM   1876  CG   ASP A 243     -27.032   -8.665  -27.392  1.00 23.99           A
ATOM   1877  OD1  ASP A 243     -25.841   -9.016  -27.513  1.00 23.11           A
ATOM   1878  OD2  ASP A 243     -27.923   -9.009  -28.204  1.00 25.61           A
ATOM   1879  C    ASP A 243     -25.164   -6.810  -25.884  1.00 22.10           A
ATOM   1880  O    ASP A 243     -25.369   -5.814  -26.583  1.00 20.96           A
ATOM   1881  N    TYR A 244     -23.946   -7.307  -25.690  1.00 20.24           A
ATOM   1882  CA   TYR A 244     -22.770   -6.623  -26.253  1.00 19.79           A
ATOM   1883  CB   TYR A 244     -21.471   -7.367  -25.865  1.00 18.34           A
ATOM   1884  CG   TYR A 244     -21.137   -8.593  -26.702  1.00 19.53           A
ATOM   1885  CD1  TYR A 244     -20.406   -8.482  -27.886  1.00 17.48           A
ATOM   1886  CE1  TYR A 244     -20.127   -9.596  -28.685  1.00 19.93           A
ATOM   1887  CD2  TYR A 244     -21.593   -9.867  -26.332  1.00 19.90           A
ATOM   1888  CE2  TYR A 244     -21.327  -10.988  -27.129  1.00 19.80           A
ATOM   1889  CZ   TYR A 244     -20.596  -10.862  -28.296  1.00 20.77           A
ATOM   1890  OH   TYR A 244     -20.321  -11.983  -29.074  1.00 23.28           A
ATOM   1891  C    TYR A 244     -22.837   -6.509  -27.775  1.00 20.37           A
ATOM   1892  O    TYR A 244     -22.257   -5.614  -28.359  1.00 19.31           A
ATOM   1893  N    ARG A 245     -23.534   -7.435  -28.413  1.00 19.69           A
ATOM   1894  CA   ARG A 245     -23.627   -7.419  -29.862  1.00 22.13           A
ATOM   1895  CB   ARG A 245     -24.410   -8.644  -30.335  1.00 22.26           A
ATOM   1896  CG   ARG A 245     -23.819   -9.936  -29.832  1.00 24.54           A
ATOM   1897  CD   ARG A 245     -24.691  -11.115  -30.214  1.00 27.20           A
ATOM   1898  NE   ARG A 245     -24.296  -12.348  -29.532  1.00 28.66           A
ATOM   1899  CZ   ARG A 245     -24.422  -12.577  -28.226  1.00 27.22           A
ATOM   1900  NH1  ARG A 245     -24.931  -11.658  -27.413  1.00 26.49           A
ATOM   1901  NH2  ARG A 245     -24.061  -13.756  -27.734  1.00 27.45           A
ATOM   1902  C    ARG A 245     -24.284   -6.151  -30.393  1.00 22.87           A
ATOM   1903  O    ARG A 245     -23.999   -5.734  -31.526  1.00 23.81           A
ATOM   1904  N    ARG A 246     -25.168   -5.559  -29.592  1.00 22.53           A
ATOM   1905  CA   ARG A 246     -25.866   -4.326  -29.978  1.00 23.83           A
ATOM   1906  CB   ARG A 246     -27.271   -4.311  -29.361  1.00 23.77           A
ATOM   1907  CG   ARG A 246     -28.060   -5.575  -29.729  1.00 27.25           A
ATOM   1908  CD   ARG A 246     -29.543   -5.486  -29.396  1.00 29.82           A
ATOM   1909  NE   ARG A 246     -30.202   -4.515  -30.263  1.00 32.86           A
ATOM   1910  CZ   ARG A 246     -31.509   -4.274  -30.246  1.00 34.97           A
ATOM   1911  NH1  ARG A 246     -32.296   -4.935  -29.410  1.00 35.99           A
ATOM   1912  NH2  ARG A 246     -32.030   -3.375  -31.071  1.00 36.57           A
ATOM   1913  C    ARG A 246     -25.093   -3.074  -29.554  1.00 22.99           A
ATOM   1914  O    ARG A 246     -25.477   -1.950  -29.900  1.00 23.88           A
ATOM   1915  N    VAL A 247     -24.027   -3.274  -28.773  1.00 21.04           A
ATOM   1916  CA   VAL A 247     -23.177   -2.178  -28.299  1.00 20.18           A
ATOM   1917  CB   VAL A 247     -22.685   -2.447  -26.850  1.00 19.13           A
ATOM   1918  CG1  VAL A 247     -21.670   -1.393  -26.413  1.00 20.39           A
ATOM   1919  CG2  VAL A 247     -23.885   -2.440  -25.907  1.00 21.24           A
ATOM   1920  C    VAL A 247     -21.979   -1.976  -29.241  1.00 19.85           A
ATOM   1921  O    VAL A 247     -21.472   -0.844  -29.390  1.00 20.50           A
ATOM   1922  N    LEU A 248     -21.516   -3.048  -29.877  1.00 19.31           A
ATOM   1923  CA   LEU A 248     -20.397   -2.896  -30.804  1.00 21.46           A
ATOM   1924  CB   LEU A 248     -20.015   -4.239  -31.435  1.00 23.15           A
ATOM   1925  CG   LEU A 248     -19.568   -5.316  -30.439  1.00 23.14           A
ATOM   1926  CD1  LEU A 248     -19.300   -6.602  -31.217  1.00 26.15           A
ATOM   1927  CD2  LEU A 248     -18.337   -4.866  -29.663  1.00 24.04           A
ATOM   1928  C    LEU A 248     -20.810   -1.939  -31.923  1.00 22.45           A
ATOM   1929  O    LEU A 248     -21.902   -2.054  -32.474  1.00 22.72           A
ATOM   1930  N    PRO A 249     -19.946   -0.977  -32.273  1.00 21.88           A
ATOM   1931  CD   PRO A 249     -18.668   -0.598  -31.642  1.00 20.48           A
ATOM   1932  CA   PRO A 249     -20.321   -0.052  -33.353  1.00 23.12           A
ATOM   1933  CB   PRO A 249     -19.090    0.843  -33.496  1.00 23.55           A
ATOM   1934  CG   PRO A 249     -18.466    0.807  -32.149  1.00 22.18           A
ATOM   1935  C    PRO A 249     -20.613   -0.821  -34.643  1.00 25.18           A
ATOM   1936  O    PRO A 249     -19.874   -1.745  -35.018  1.00 25.69           A
ATOM   1937  N    LYS A 250     -21.675   -0.416  -35.333  1.00 26.79           A
ATOM   1938  CA   LYS A 250     -22.112   -1.071  -36.567  1.00 30.40           A
ATOM   1939  CB   LYS A 250     -23.408   -0.429  -37.065  1.00 31.64           A
ATOM   1940  CG   LYS A 250     -24.527   -0.363  -36.043  1.00 36.92           A
ATOM   1941  CD   LYS A 250     -25.774    0.328  -36.638  1.00 40.37           A
ATOM   1942  CE   LYS A 250     -25.511    1.793  -37.053  1.00 41.65           A
ATOM   1943  NZ   LYS A 250     -26.750    2.478  -37.569  1.00 42.08           A
ATOM   1944  C    LYS A 250     -21.121   -1.074  -37.714  1.00 30.98           A
ATOM   1945  O    LYS A 250     -20.828   -2.113  -38.296  1.00 32.45           A
ATOM   1946  N    ASN A 251     -20.612    0.098  -38.055  1.00 31.28           A
ATOM   1947  CA   ASN A 251     -19.680    0.188  -39.161  1.00 32.02           A
ATOM   1948  CB   ASN A 251     -20.420    0.641  -40.431  1.00 34.75           A
ATOM   1949  CG   ASN A 251     -21.586   -0.287  -40.805  1.00 37.52           A
ATOM   1950  OD1  ASN A 251     -22.755    0.120  -40.783  1.00 39.85           A
ATOM   1951  ND2  ASN A 251     -21.268   -1.535  -41.154  1.00 38.31           A
ATOM   1952  C    ASN A 251     -18.563    1.164  -38.809  1.00 30.42           A
ATOM   1953  O    ASN A 251     -18.527    2.299  -39.297  1.00 31.94           A
ATOM   1954  N    PRO A 252     -17.649    0.734  -37.928  1.00 28.72           A
ATOM   1955  CD   PRO A 252     -17.660   -0.563  -37.218  1.00 27.35           A
ATOM   1956  CA   PRO A 252     -16.517    1.563  -37.492  1.00 27.89           A
ATOM   1957  CB   PRO A 252     -16.132    0.917  -36.167  1.00 26.42           A
ATOM   1958  CG   PRO A 252     -16.328   -0.561  -36.468  1.00 27.43           A
ATOM   1959  C    PRO A 252     -15.410    1.473  -38.539  1.00 29.12           A
ATOM   1960  O    PRO A 252     -14.323    0.959  -38.263  1.00 29.62           A
ATOM   1961  N    ASP A 253     -15.716    2.003  -39.723  1.00 30.27           A
ATOM   1962  CA   ASP A 253     -14.869    1.991  -40.920  1.00 31.73           A
ATOM   1963  CB   ASP A 253     -15.625    2.669  -42.079  1.00 35.32           A
ATOM   1964  CG   ASP A 253     -15.798    4.184  -41.878  1.00 39.92           A
ATOM   1965  OD1  ASP A 253     -16.335    4.607  -40.819  1.00 42.78           A
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Figure 1 (continued 20)

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ATOM  1966  OD2 ASP A 253   -15.400   4.962 -42.784  1.00 41.27    A
ATOM  1967  C   ASP A 253   -13.467   2.586 -40.870  1.00 30.28    A
ATOM  1968  O   ASP A 253   -12.578   2.126 -41.600  1.00 31.43    A
ATOM  1969  N   LYS A 254   -13.277   3.606 -40.039  1.00 27.06    A
ATOM  1970  CA  LYS A 254   -11.991   4.285 -39.932  1.00 24.92    A
ATOM  1971  CB  LYS A 254   -12.232   5.728 -39.494  1.00 24.91    A
ATOM  1972  CG  LYS A 254   -13.148   6.522 -40.421  1.00 27.11    A
ATOM  1973  CD  LYS A 254   -13.379   7.918 -39.844  1.00 29.21    A
ATOM  1974  CE  LYS A 254   -14.184   8.777 -40.825  1.00 32.00    A
ATOM  1975  NZ  LYS A 254   -15.470   8.129 -41.185  1.00 34.43    A
ATOM  1976  C   LYS A 254   -11.094   3.553 -38.930  1.00 22.15    A
ATOM  1977  O   LYS A 254   -11.328   3.610 -37.730  1.00 22.88    A
ATOM  1978  N   HIS A 255   -10.067   2.884 -39.434  1.00 21.10    A
ATOM  1979  CA  HIS A 255    -9.165   2.101 -38.598  1.00 21.30    A
ATOM  1980  CB  HIS A 255    -8.939   0.721 -39.214  1.00 24.75    A
ATOM  1981  CG  HIS A 255   -10.171  -0.127 -39.294  1.00 26.36    A
ATOM  1982  CD2 HIS A 255   -10.391  -1.313 -39.905  1.00 28.26    A
ATOM  1983  ND1 HIS A 255   -11.359   0.219 -38.684  1.00 29.22    A
ATOM  1984  CE1 HIS A 255   -12.261  -0.718 -38.922  1.00 29.44    A
ATOM  1985  NE2 HIS A 255   -11.699  -1.658 -39.660  1.00 31.29    A
ATOM  1986  C   HIS A 255    -7.798   2.727 -38.381  1.00 20.47    A
ATOM  1987  O   HIS A 255    -7.045   2.966 -39.331  1.00 19.05    A
ATOM  1988  N   LEU A 256    -7.449   2.930 -37.120  1.00 18.43    A
ATOM  1989  CA  LEU A 256    -6.148   3.491 -36.778  1.00 18.02    A
ATOM  1990  CB  LEU A 256    -6.351   4.753 -35.927  1.00 19.89    A
ATOM  1991  CG  LEU A 256    -5.142   5.472 -35.324  1.00 22.32    A
ATOM  1992  CD1 LEU A 256    -5.493   6.944 -35.096  1.00 24.64    A
ATOM  1993  CD2 LEU A 256    -4.737   4.798 -34.007  1.00 23.40    A
ATOM  1994  C   LEU A 256    -5.368   2.452 -35.962  1.00 18.20    A
ATOM  1995  O   LEU A 256    -5.921   1.857 -35.042  1.00 17.77    A
ATOM  1996  N   GLU A 257    -4.099   2.224 -36.298  1.00 16.89    A
ATOM  1997  CA  GLU A 257    -3.295   1.292 -35.505  1.00 17.61    A
ATOM  1998  CB  GLU A 257    -2.702   0.186 -36.378  1.00 19.65    A
ATOM  1999  CG  GLU A 257    -1.850  -0.790 -35.585  1.00 25.47    A
ATOM  2000  CD  GLU A 257    -1.391  -1.990 -36.398  1.00 28.58    A
ATOM  2001  OE1 GLU A 257    -0.339  -2.592 -36.024  1.00 30.83    A
ATOM  2002  OE2 GLU A 257    -2.089  -2.333 -37.394  1.00 26.86    A
ATOM  2003  C   GLU A 257    -2.182   2.113 -34.861  1.00 17.45    A
ATOM  2004  O   GLU A 257    -1.570   2.963 -35.515  1.00 16.51    A
ATOM  2005  N   ALA A 258    -1.932   1.863 -33.579  1.00 17.17    A
ATOM  2006  CA  ALA A 258    -0.906   2.593 -32.830  1.00 17.02    A
ATOM  2007  CB  ALA A 258    -1.584   3.719 -32.020  1.00 18.18    A
ATOM  2008  C   ALA A 258    -0.172   1.666 -31.864  1.00 18.03    A
ATOM  2009  O   ALA A 258    -0.738   0.663 -31.398  1.00 17.35    A
ATOM  2010  N   GLY A 259     1.085   2.001 -31.571  1.00 16.83    A
ATOM  2011  CA  GLY A 259     1.860   1.248 -30.598  1.00 16.02    A
ATOM  2012  C   GLY A 259     1.145   1.382 -29.257  1.00 16.37    A
ATOM  2013  O   GLY A 259     0.829   2.476 -28.834  1.00 15.32    A
ATOM  2014  N   CYS A 260     0.894   0.270 -28.576  1.00 14.83    A
ATOM  2015  CA  CYS A 260     0.143   0.338 -27.323  1.00 14.73    A
ATOM  2016  CB  CYS A 260    -0.107  -1.069 -26.807  1.00 13.90    A
ATOM  2017  SG  CYS A 260    -1.234  -1.099 -25.368  1.00 18.12    A
ATOM  2018  C   CYS A 260     0.806   1.179 -26.253  1.00 14.83    A
ATOM  2019  O   CYS A 260     0.159   2.047 -25.640  1.00 15.46    A
ATOM  2020  N   ASP A 261     2.096   0.921 -26.017  1.00 15.27    A
ATOM  2021  CA  ASP A 261     2.834   1.655 -24.977  1.00 17.33    A
ATOM  2022  CB  ASP A 261     4.276   1.123 -24.801  1.00 18.87    A
ATOM  2023  CG  ASP A 261     5.188   2.109 -24.002  1.00 25.56    A
ATOM  2024  OD1 ASP A 261     5.948   2.946 -24.607  1.00 27.19    A
ATOM  2025  OD2 ASP A 261     5.128   2.056 -22.758  1.00 23.92    A
ATOM  2026  C   ASP A 261     2.924   3.126 -25.321  1.00 15.30    A
ATOM  2027  O   ASP A 261     2.689   3.977 -24.457  1.00 16.28    A
ATOM  2028  N   LEU A 262     3.263   3.435 -26.566  1.00 15.05    A
ATOM  2029  CA  LEU A 262     3.379   4.835 -26.940  1.00 14.87    A
ATOM  2030  CB  LEU A 262     3.900   4.980 -28.365  1.00 16.84    A
ATOM  2031  CG  LEU A 262     5.392   4.695 -28.564  1.00 19.33    A
ATOM  2032  CD1 LEU A 262     5.705   4.835 -30.069  1.00 20.64    A
ATOM  2033  CD2 LEU A 262     6.233   5.673 -27.721  1.00 19.45    A
ATOM  2034  C   LEU A 262     2.041   5.563 -26.782  1.00 15.27    A
ATOM  2035  O   LEU A 262     2.003   6.712 -26.332  1.00 15.81    A
ATOM  2036  N   LEU A 263     0.949   4.912 -27.161  1.00 13.33    A
ATOM  2037  CA  LEU A 263    -0.352   5.560 -26.991  1.00 13.53    A
ATOM  2038  CB  LEU A 263    -1.447   4.721 -27.673  1.00 13.61    A
ATOM  2039  CG  LEU A 263    -2.885   5.243 -27.627  1.00 16.53    A
ATOM  2040  CD1 LEU A 263    -2.965   6.612 -28.293  1.00 17.32    A
ATOM  2041  CD2 LEU A 263    -3.785   4.257 -28.319  1.00 15.91    A
ATOM  2042  C   LEU A 263    -0.658   5.736 -25.491  1.00 14.38    A
ATOM  2043  O   LEU A 263    -1.177   6.774 -25.064  1.00 13.47    A
ATOM  2044  N   LYS A 264    -0.372   4.719 -24.680  1.00 13.04    A
ATOM  2045  CA  LYS A 264    -0.655   4.778 -23.255  1.00 14.11    A
ATOM  2046  CB  LYS A 264    -0.299   3.420 -22.644  1.00 15.66    A
ATOM  2047  CG  LYS A 264    -0.539   3.304 -21.166  1.00 22.39    A
ATOM  2048  CD  LYS A 264    -0.002   1.952 -20.693  1.00 25.24    A
ATOM  2049  CE  LYS A 264    -0.624   0.789 -21.454  1.00 28.82    A
ATOM  2050  NZ  LYS A 264    -0.186  -0.554 -20.920  1.00 32.53    A
ATOM  2051  C   LYS A 264     0.110   5.920 -22.559  1.00 13.53    A
ATOM  2052  O   LYS A 264    -0.474   6.700 -21.798  1.00 13.19    A
ATOM  2053  N   GLN A 265     1.397   6.058 -22.861  1.00 12.97    A
ATOM  2054  CA  GLN A 265     2.167   7.097 -22.192  1.00 13.73    A
ATOM  2055  CB  GLN A 265     3.668   6.889 -22.418  1.00 14.32    A
ATOM  2056  CG  GLN A 265     4.187   5.506 -21.997  1.00 15.83    A
ATOM  2057  CD  GLN A 265     3.603   5.004 -20.674  1.00 16.85    A
ATOM  2058  OE1 GLN A 265     3.288   5.773 -19.777  1.00 18.55    A
ATOM  2059  NE2 GLN A 265     3.473   3.687 -20.551  1.00 19.72    A
ATOM  2060  C   GLN A 265     1.789   8.491 -22.685  1.00 13.91    A
ATOM  2061  O   GLN A 265     1.882   9.454 -21.921  1.00 14.00    A
ATOM  2062  N   ALA A 266     1.367   8.598 -23.947  1.00 12.99    A
ATOM  2063  CA  ALA A 266     0.949   9.897 -24.477  1.00 12.33    A
ATOM  2064  CB  ALA A 266     0.735   9.820 -25.983  1.00 13.59    A
ATOM  2065  C   ALA A 266    -0.356  10.311 -23.760  1.00 14.35    A
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Figure 1 (continued 21)

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ATOM   2066  O   ALA A 266     -0.533  11.459 -23.384  1.00 12.81      A
ATOM   2067  N   PHE A 267     -1.264   9.349 -23.570  1.00 12.67      A
ATOM   2068  CA  PHE A 267     -2.497   9.629 -22.832  1.00 14.64      A
ATOM   2069  CB  PHE A 267     -3.412   8.384 -22.796  1.00 14.10      A
ATOM   2070  CG  PHE A 267     -4.587   8.456 -23.724  1.00 17.70      A
ATOM   2071  CD1 PHE A 267     -5.889   8.659 -23.221  1.00 16.72      A
ATOM   2072  CD2 PHE A 267     -4.418   8.320 -25.085  1.00 16.56      A
ATOM   2073  CE1 PHE A 267     -6.996   8.726 -24.090  1.00 18.75      A
ATOM   2074  CE2 PHE A 267     -5.546   8.387 -25.986  1.00 17.43      A
ATOM   2075  CZ  PHE A 267     -6.830   8.592 -25.468  1.00 18.69      A
ATOM   2076  C   PHE A 267     -2.183  10.001 -21.400  1.00 13.98      A
ATOM   2077  O   PHE A 267     -2.749  10.943 -20.853  1.00 13.44      A
ATOM   2078  N   ALA A 268     -1.294   9.225 -20.777  1.00 13.32      A
ATOM   2079  CA  ALA A 268     -0.945   9.470 -19.386  1.00 13.98      A
ATOM   2080  CB  ALA A 268     -0.017   8.371 -18.892  1.00 13.57      A
ATOM   2081  C   ALA A 268     -0.312  10.844 -19.175  1.00 11.09      A
ATOM   2082  O   ALA A 268     -0.648  11.560 -18.212  1.00 12.76      A
ATOM   2083  N   ARG A 269      0.568  11.264 -20.087  1.00 10.81      A
ATOM   2084  CA  ARG A 269      1.206  12.564 -19.928  1.00  9.72      A
ATOM   2085  CB  ARG A 269      2.418  12.695 -20.883  1.00 10.65      A
ATOM   2086  CG  ARG A 269      3.640  11.953 -20.390  1.00 10.06      A
ATOM   2087  CD  ARG A 269      4.892  12.362 -21.249  1.00 10.44      A
ATOM   2088  NE  ARG A 269      4.685  12.077 -22.658  1.00  9.73      A
ATOM   2089  CZ  ARG A 269      4.963  10.922 -23.254  1.00  9.84      A
ATOM   2090  NH1 ARG A 269      5.499   9.908 -22.580  1.00 11.65      A
ATOM   2091  NH2 ARG A 269      4.653  10.760 -24.520  1.00 10.88      A
ATOM   2092  C   ARG A 269      0.217  13.699 -20.230  1.00 10.56      A
ATOM   2093  O   ARG A 269      0.169  14.656 -19.489  1.00 11.75      A
ATOM   2094  N   ALA A 270     -0.558  13.569 -21.309  1.00  9.54      A
ATOM   2095  CA  ALA A 270     -1.515  14.637 -21.642  1.00 10.89      A
ATOM   2096  CB  ALA A 270     -2.260  14.289 -22.911  1.00 13.90      A
ATOM   2097  C   ALA A 270     -2.506  14.807 -20.483  1.00 11.27      A
ATOM   2098  O   ALA A 270     -2.874  15.950 -20.153  1.00 12.70      A
ATOM   2099  N   ALA A 271     -2.903  13.697 -19.871  1.00 13.03      A
ATOM   2100  CA  ALA A 271     -3.876  13.755 -18.758  1.00 13.13      A
ATOM   2101  CB  ALA A 271     -4.215  12.366 -18.293  1.00 12.98      A
ATOM   2102  C   ALA A 271     -3.481  14.622 -17.569  1.00 12.80      A
ATOM   2103  O   ALA A 271     -4.354  15.128 -16.831  1.00 12.02      A
ATOM   2104  N   ILE A 272     -2.177  14.869 -17.385  1.00 11.81      A
ATOM   2105  CA  ILE A 272     -1.711  15.689 -16.290  1.00 10.77      A
ATOM   2106  CB  ILE A 272     -0.166  15.743 -16.339  1.00 10.82      A
ATOM   2107  CG2 ILE A 272      0.362  16.726 -15.319  1.00 12.90      A
ATOM   2108  CG1 ILE A 272      0.353  14.310 -16.155  1.00 10.24      A
ATOM   2109  CD1 ILE A 272      1.872  14.133 -16.554  1.00 12.64      A
ATOM   2110  C   ILE A 272     -2.287  17.132 -16.343  1.00 11.14      A
ATOM   2111  O   ILE A 272     -2.512  17.770 -15.302  1.00 13.87      A
ATOM   2112  N   LEU A 273     -2.507  17.638 -17.560  1.00 11.27      A
ATOM   2113  CA  LEU A 273     -3.035  18.998 -17.702  1.00 11.91      A
ATOM   2114  CB  LEU A 273     -2.145  19.857 -18.640  1.00 11.25      A
ATOM   2115  CG  LEU A 273     -0.698  19.888 -18.117  1.00 12.82      A
ATOM   2116  CD1 LEU A 273      0.147  20.788 -19.043  1.00 14.39      A
ATOM   2117  CD2 LEU A 273     -0.605  20.368 -16.660  1.00 13.33      A
ATOM   2118  C   LEU A 273     -4.479  19.034 -18.155  1.00 13.42      A
ATOM   2119  O   LEU A 273     -4.918  20.032 -18.737  1.00 13.16      A
ATOM   2120  N   SER A 274     -5.185  17.936 -17.879  1.00 13.18      A
ATOM   2121  CA  SER A 274     -6.625  17.884 -18.193  1.00 16.03      A
ATOM   2122  CB  SER A 274     -7.040  16.461 -18.570  1.00 15.17      A
ATOM   2123  OG  SER A 274     -6.960  15.560 -17.484  1.00 16.66      A
ATOM   2124  C   SER A 274     -7.363  18.365 -16.933  1.00 15.64      A
ATOM   2125  O   SER A 274     -6.734  18.682 -15.911  1.00 17.51      A
ATOM   2126  N   ASN A 275     -8.696  18.484 -16.988  1.00 14.62      A
ATOM   2127  CA  ASN A 275     -9.397  18.935 -15.774  1.00 17.24      A
ATOM   2128  CB  ASN A 275    -10.872  19.209 -16.082  1.00 16.46      A
ATOM   2129  CG  ASN A 275    -11.590  19.909 -14.923  1.00 18.43      A
ATOM   2130  OD1 ASN A 275    -11.704  19.358 -13.827  1.00 22.10      A
ATOM   2131  ND2 ASN A 275    -12.067  21.138 -15.170  1.00 18.70      A
ATOM   2132  C   ASN A 275     -9.307  17.879 -14.662  1.00 18.08      A
ATOM   2133  O   ASN A 275     -9.747  16.752 -14.843  1.00 17.91      A
ATOM   2134  N   GLU A 276     -8.718  18.235 -13.523  1.00 21.67      A
ATOM   2135  CA  GLU A 276     -8.539  17.290 -12.401  1.00 25.21      A
ATOM   2136  CB  GLU A 276     -7.902  17.993 -11.189  1.00 30.38      A
ATOM   2137  CG  GLU A 276     -6.672  18.817 -11.475  1.00 37.32      A
ATOM   2138  CD  GLU A 276     -5.401  17.997 -11.551  1.00 42.05      A
ATOM   2139  OE1 GLU A 276     -5.122  17.211 -10.603  1.00 44.93      A
ATOM   2140  OE2 GLU A 276     -4.667  18.154 -12.553  1.00 45.14      A
ATOM   2141  C   GLU A 276     -9.796  16.578 -11.907  1.00 26.06      A
ATOM   2142  O   GLU A 276     -9.724  15.425 -11.457  1.00 24.42      A
ATOM   2143  N   LYS A 277    -10.946  17.254 -11.984  1.00 25.49      A
ATOM   2144  CA  LYS A 277    -12.218  16.681 -11.525  1.00 27.23      A
ATOM   2145  CB  LYS A 277    -13.203  17.806 -11.157  1.00 29.01      A
ATOM   2146  CG  LYS A 277    -12.699  18.790 -10.106  1.00 33.53      A
ATOM   2147  CD  LYS A 277    -12.724  18.215  -8.698  1.00 36.20      A
ATOM   2148  CE  LYS A 277    -12.225  19.257  -7.698  1.00 37.26      A
ATOM   2149  NZ  LYS A 277    -12.511  18.878  -6.273  1.00 39.68      A
ATOM   2150  C   LYS A 277    -12.884  15.775 -12.562  1.00 25.59      A
ATOM   2151  O   LYS A 277    -13.731  14.943 -12.220  1.00 25.69      A
ATOM   2152  N   PHE A 278    -12.498  15.921 -13.825  1.00 24.84      A
ATOM   2153  CA  PHE A 278    -13.092  15.122 -14.896  1.00 23.67      A
ATOM   2154  CB  PHE A 278    -14.380  15.816 -15.313  1.00 25.91      A
ATOM   2155  CG  PHE A 278    -15.369  14.929 -15.984  1.00 29.29      A
ATOM   2156  CD1 PHE A 278    -15.276  13.538 -15.875  1.00 30.58      A
ATOM   2157  CD2 PHE A 278    -16.425  15.485 -16.705  1.00 30.56      A
ATOM   2158  CE1 PHE A 278    -16.220  12.710 -16.471  1.00 32.00      A
ATOM   2159  CE2 PHE A 278    -17.383  14.658 -17.310  1.00 31.23      A
ATOM   2160  CZ  PHE A 278    -17.278  13.270 -17.191  1.00 33.81      A
ATOM   2161  C   PHE A 278    -12.076  15.063 -16.050  1.00 21.94      A
ATOM   2162  O   PHE A 278    -12.137  15.874 -16.975  1.00 21.84      A
ATOM   2163  N   ARG A 279    -11.154  14.096 -15.989  1.00 19.13      A
ATOM   2164  CA  ARG A 279    -10.063  14.036 -16.962  1.00 18.33      A
ATOM   2165  CB  ARG A 279     -8.844  13.272 -16.376  1.00 18.78      A
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Figure 1 (continued 22)

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ATOM   2166  CG   ARG A 279     -8.186  13.898 -15.146  1.00 23.64      A
ATOM   2167  CD   ARG A 279     -6.825  13.215 -14.864  1.00 26.45      A
ATOM   2168  NE   ARG A 279     -6.393  13.464 -13.493  1.00 31.51      A
ATOM   2169  CZ   ARG A 279     -5.871  14.612 -13.074  1.00 33.69      A
ATOM   2170  NH1  ARG A 279     -5.708  15.616 -13.934  1.00 35.31      A
ATOM   2171  NH2  ARG A 279     -5.529  14.763 -11.792  1.00 33.02      A
ATOM   2172  C    ARG A 279    -10.359  13.458 -18.314  1.00 14.43      A
ATOM   2173  O    ARG A 279    -10.674  12.294 -18.433  1.00 16.83      A
ATOM   2174  N    GLY A 280    -10.222  14.291 -19.333  1.00 14.30      A
ATOM   2175  CA   GLY A 280    -10.420  13.855 -20.696  1.00 13.40      A
ATOM   2176  C    GLY A 280     -9.408  14.511 -21.632  1.00 12.18      A
ATOM   2177  O    GLY A 280     -8.837  15.565 -21.311  1.00 13.28      A
ATOM   2178  N    VAL A 281     -9.193  13.896 -22.795  1.00 13.04      A
ATOM   2179  CA   VAL A 281     -8.254  14.440 -23.796  1.00 12.38      A
ATOM   2180  CB   VAL A 281     -6.960  13.531 -23.909  1.00 13.51      A
ATOM   2181  CG1  VAL A 281     -6.103  13.679 -22.671  1.00 12.12      A
ATOM   2182  CG2  VAL A 281     -7.362  12.090 -24.098  1.00 15.36      A
ATOM   2183  C    VAL A 281     -8.927  14.482 -25.165  1.00 12.53      A
ATOM   2184  O    VAL A 281     -9.866  13.716 -25.457  1.00 13.70      A
ATOM   2185  N    ARG A 282     -8.453  15.380 -26.026  1.00 11.74      A
ATOM   2186  CA   ARG A 282     -8.987  15.486 -27.364  1.00 13.08      A
ATOM   2187  CB   ARG A 282     -9.165  16.947 -27.763  1.00 16.93      A
ATOM   2188  CG   ARG A 282     -9.831  17.086 -29.125  1.00 25.93      A
ATOM   2189  CD   ARG A 282    -11.067  18.017 -29.069  1.00 33.09      A
ATOM   2190  NE   ARG A 282    -11.959  17.716 -27.940  1.00 37.56      A
ATOM   2191  CZ   ARG A 282    -13.099  17.025 -28.030  1.00 38.42      A
ATOM   2192  NH1  ARG A 282    -13.519  16.552 -29.200  1.00 38.59      A
ATOM   2193  NH2  ARG A 282    -13.822  16.805 -26.940  1.00 38.91      A
ATOM   2194  C    ARG A 282     -8.029  14.816 -28.330  1.00 14.43      A
ATOM   2195  O    ARG A 282     -6.815  15.031 -28.216  1.00 16.20      A
ATOM   2196  N    LEU A 283     -8.566  14.022 -29.267  1.00 12.40      A
ATOM   2197  CA   LEU A 283     -7.754  13.341 -30.279  1.00 13.04      A
ATOM   2198  CB   LEU A 283     -8.052  11.840 -30.387  1.00 14.68      A
ATOM   2199  CG   LEU A 283     -7.290  10.870 -29.488  1.00 17.14      A
ATOM   2200  CD1  LEU A 283     -7.408  11.334 -28.017  1.00 18.12      A
ATOM   2201  CD2  LEU A 283     -7.795   9.422 -29.716  1.00 17.55      A
ATOM   2202  C    LEU A 283     -8.039  13.920 -31.638  1.00 15.68      A
ATOM   2203  O    LEU A 283     -9.192  14.041 -32.036  1.00 15.80      A
ATOM   2204  N    TYR A 284     -6.988  14.308 -32.338  1.00 13.31      A
ATOM   2205  CA   TYR A 284     -7.186  14.776 -33.696  1.00 14.87      A
ATOM   2206  CB   TYR A 284     -6.561  16.144 -33.942  1.00 14.87      A
ATOM   2207  CG   TYR A 284     -7.063  16.684 -35.265  1.00 16.70      A
ATOM   2208  CD1  TYR A 284     -8.155  17.562 -35.312  1.00 18.02      A
ATOM   2209  CE1  TYR A 284     -8.709  17.978 -36.542  1.00 19.42      A
ATOM   2210  CD2  TYR A 284     -6.532  16.232 -36.466  1.00 16.24      A
ATOM   2211  CE2  TYR A 284     -7.077  16.638 -37.685  1.00 18.82      A
ATOM   2212  CZ   TYR A 284     -8.165  17.514 -37.713  1.00 19.97      A
ATOM   2213  OH   TYR A 284     -8.692  17.919 -38.933  1.00 20.44      A
ATOM   2214  C    TYR A 284     -6.517  13.731 -34.561  1.00 14.90      A
ATOM   2215  O    TYR A 284     -5.293  13.519 -34.503  1.00 15.97      A
ATOM   2216  N    VAL A 285     -7.320  13.050 -35.369  1.00 14.02      A
ATOM   2217  CA   VAL A 285     -6.768  12.007 -36.209  1.00 14.58      A
ATOM   2218  CB   VAL A 285     -7.728  10.797 -36.264  1.00 16.41      A
ATOM   2219  CG1  VAL A 285     -7.087   9.678 -37.030  1.00 19.28      A
ATOM   2220  CG2  VAL A 285     -8.053  10.335 -34.836  1.00 17.87      A
ATOM   2221  C    VAL A 285     -6.566  12.520 -37.615  1.00 13.95      A
ATOM   2222  O    VAL A 285     -7.463  13.109 -38.191  1.00 16.55      A
ATOM   2223  N    SER A 286     -5.376  12.297 -38.168  1.00 13.98      A
ATOM   2224  CA   SER A 286     -5.094  12.724 -39.555  1.00 13.75      A
ATOM   2225  CB   SER A 286     -4.453  14.129 -39.576  1.00 15.23      A
ATOM   2226  OG   SER A 286     -3.165  14.108 -38.984  1.00 16.02      A
ATOM   2227  C    SER A 286     -4.198  11.659 -40.201  1.00 15.02      A
ATOM   2228  O    SER A 286     -3.859  10.670 -39.558  1.00 15.90      A
ATOM   2229  N    GLU A 287     -3.806  11.824 -41.465  1.00 16.50      A
ATOM   2230  CA   GLU A 287     -3.006  10.788 -42.132  1.00 17.09      A
ATOM   2231  CB   GLU A 287     -2.655  11.245 -43.568  1.00 20.13      A
ATOM   2232  CG   GLU A 287     -2.338  10.108 -44.526  1.00 25.94      A
ATOM   2233  CD   GLU A 287     -3.594   9.464 -45.178  1.00 31.11      A
ATOM   2234  OE1  GLU A 287     -4.753   9.927 -44.995  1.00 33.30      A
ATOM   2235  OE2  GLU A 287     -3.410   8.466 -45.909  1.00 36.38     |A
ATOM   2236  C    GLU A 287     -1.752  10.371 -41.363  1.00 17.84      A
ATOM   2237  O    GLU A 287     -0.845  11.172 -41.104  1.00 16.79      A
ATOM   2238  N    ASN A 288     -1.734   9.100 -40.955  1.00 15.55      A
ATOM   2239  CA   ASN A 288     -0.648   8.524 -40.188  1.00 15.15      A
ATOM   2240  CB   ASN A 288      0.548   8.265 -41.097  1.00 18.14      A
ATOM   2241  CG   ASN A 288      0.272   7.178 -42.139  1.00 19.57      A
ATOM   2242  OD1  ASN A 288      0.911   7.151 -43.202  1.00 24.08      A
ATOM   2243  ND2  ASN A 288     -0.643   6.263 -41.837  1.00 15.66      A
ATOM   2244  C    ASN A 288     -0.221   9.333 -38.969  1.00 14.72      A
ATOM   2245  O    ASN A 288      0.933   9.275 -38.548  1.00 15.32      A
ATOM   2246  N    GLN A 289     -1.149  10.063 -38.380  1.00 12.97      A
ATOM   2247  CA   GLN A 289     -0.790  10.867 -37.209  1.00 13.76      A
ATOM   2248  CB   GLN A 289     -0.352  12.282 -37.632  1.00 14.58      A
ATOM   2249  CG   GLN A 289      0.205  13.125 -36.486  1.00 15.69      A
ATOM   2250  CD   GLN A 289      0.526  14.534 -36.923  1.00 19.41      A
ATOM   2251  OE1  GLN A 289     -0.299  15.468 -36.764  1.00 22.72      A
ATOM   2252  NE2  GLN A 289      1.714  14.705 -37.504  1.00 20.35      A
ATOM   2253  C    GLN A 289     -1.906  11.022 -36.223  1.00 15.19      A
ATOM   2254  O    GLN A 289     -3.074  11.137 -36.603  1.00 14.85      A
ATOM   2255  N    LEU A 290     -1.554  11.041 -34.941  1.00 13.50      A
ATOM   2256  CA   LEU A 290     -2.559  11.268 -33.903  1.00 13.78      A
ATOM   2257  CB   LEU A 290     -2.738  10.022 -33.017  1.00 15.99      A
ATOM   2258  CG   LEU A 290     -3.770  10.099 -31.894  1.00 18.63      A
ATOM   2259  CD1  LEU A 290     -5.182  10.294 -32.481  1.00 17.72      A
ATOM   2260  CD2  LEU A 290     -3.706   8.818 -31.090  1.00 17.47      A
ATOM   2261  C    LEU A 290     -2.022  12.403 -33.039  1.00 13.83      A
ATOM   2262  O    LEU A 290     -0.872  12.377 -32.625  1.00 14.65      A
ATOM   2263  N    LYS A 291     -2.864  13.395 -32.755  1.00 12.16      A
ATOM   2264  CA   LYS A 291     -2.478  14.486 -31.879  1.00 13.66      A
ATOM   2265  CB   LYS A 291     -2.713  15.847 -32.532  1.00 16.40      A
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Figure 1 (continued 23)

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ATOM   2266  CG   LYS A 291     -2.319  17.009 -31.620  1.00 19.58      A
ATOM   2267  CD   LYS A 291     -2.331  18.365 -32.360  1.00 23.93      A
ATOM   2268  CE   LYS A 291     -1.322  18.403 -33.488  1.00 28.14      A
ATOM   2269  NZ   LYS A 291     -1.660  19.396 -34.584  1.00 31.96      A
ATOM   2270  C    LYS A 291     -3.376  14.347 -30.667  1.00 14.91      A
ATOM   2271  O    LYS A 291     -4.586  14.165 -30.812  1.00 16.66      A
ATOM   2272  N    ILE A 292     -2.798  14.395 -29.480  1.00 12.63      A
ATOM   2273  CA   ILE A 292     -3.606  14.274 -28.272  1.00 12.23      A
ATOM   2274  CB   ILE A 292     -3.122  13.080 -27.435  1.00 10.96      A
ATOM   2275  CG2  ILE A 292     -3.842  13.062 -26.067  1.00 11.48      A
ATOM   2276  CG1  ILE A 292     -3.343  11.776 -28.240  1.00 13.80      A
ATOM   2277  CD1  ILE A 292     -2.721  10.538 -27.591  1.00 15.45      A
ATOM   2278  C    ILE A 292     -3.413  15.562 -27.478  1.00 14.22      A
ATOM   2279  O    ILE A 292     -2.275  15.928 -27.152  1.00 14.71      A
ATOM   2280  N    THR A 293     -4.514  16.240 -27.130  1.00 12.06      A
ATOM   2281  CA   THR A 293     -4.395  17.489 -26.392  1.00 12.49      A
ATOM   2282  CB   THR A 293     -4.757  18.694 -27.302  1.00 14.10      A
ATOM   2283  OG1  THR A 293     -6.127  18.615 -27.691  1.00 20.69      A
ATOM   2284  CG2  THR A 293     -3.957  18.676 -28.566  1.00 13.47      A
ATOM   2285  C    THR A 293     -5.284  17.512 -25.142  1.00 13.28      A
ATOM   2286  O    THR A 293     -6.324  16.840 -25.073  1.00 13.69      A
ATOM   2287  N    ALA A 294     -4.817  18.231 -24.147  1.00 11.90      A
ATOM   2288  CA   ALA A 294     -5.546  18.421 -22.880  1.00 11.99      A
ATOM   2289  CB   ALA A 294     -4.986  17.521 -21.790  1.00 14.59      A
ATOM  -2290  C    ALA A 294     -5.443  19.858 -22.433  1.00 11.96      A
ATOM   2291  O    ALA A 294     -4.440  20.536 -22.685  1.00 13.42      A
ATOM   2292  N    ASN A 295     -6.472  20.330 -21.721  1.00 13.29      A
ATOM   2293  CA   ASN A 295     -6.503  21.690 -21.209  1.00 15.53      A
ATOM   2294  CB   ASN A 295     -7.326  22.622 -22.129  1.00 20.85      A
ATOM   2295  CG   ASN A 295     -6.805  22.666 -23.539  1.00 23.25      A
ATOM   2296  OD1  ASN A 295     -6.030  23.558 -23.901  1.00 29.01      A
ATOM   2297  ND2  ASN A 295     -7.217  21.704 -24.350  1.00 25.32      A
ATOM   2298  C    ASN A 295     -7.244  21.643 -19.881  1.00 13.79      A
ATOM   2299  O    ASN A 295     -8.046  20.725 -19.625  1.00 14.51      A
ATOM   2300  N    ASN A 296     -6.970  22.631 -19.048  1.00 14.40      A
ATOM   2301  CA   ASN A 296     -7.627  22.709 -17.746  1.00 15.59      A
ATOM   2302  CB   ASN A 296     -6.711  22.122 -16.646  1.00 15.58      A
ATOM   2303  CG   ASN A 296     -5.444  22.935 -16.427  1.00 15.76      A
ATOM   2304  OD1  ASN A 296     -5.394  24.114 -16.766  1.00 15.10      A
ATOM   2305  ND2  ASN A 296     -4.415  22.304 -15.829  1.00 18.05      A
ATOM   2306  C    ASN A 296     -8.068  24.163 -17.462  1.00 16.76      A
ATOM   2307  O    ASN A 296     -7.770  25.094 -18.230  1.00 15.08      A
ATOM   2308  N    PRO A 297     -8.769  24.383 -16.344  1.00 20.01      A
ATOM   2309  CD   PRO A 297     -9.315  23.409 -15.393  1.00 21.18      A
ATOM   2310  CA   PRO A 297     -9.225  25.747 -16.039  1.00 22.92      A
ATOM   2311  CB   PRO A 297    -10.099  25.553 -14.792  1.00 23.25      A
ATOM   2312  CG   PRO A 297    -10.607  24.125 -14.971  1.00 22.77      A
ATOM   2313  C    PRO A 297     -8.127  26.786 -15.819  1.00 24.45      A
ATOM   2314  O    PRO A 297     -8.382  28.000 -15.915  1.00 27.11      A
ATOM   2315  N    GLU A 298     -6.919  26.306 -15.521  1.00 24.38      A
ATOM   2316  CA   GLU A 298     -5.767  27.174 -15.283  1.00 24.08      A
ATOM   2317  CB   GLU A 298     -4.690  26.433 -14.480  1.00 26.78      A
ATOM   2318  CG   GLU A 298     -5.007  26.166 -12.995  1.00 33.37      A
ATOM   2319  CD   GLU A 298     -5.908  24.952 -12.723  1.00 35.97      A
ATOM   2320  OE1  GLU A 298     -6.051  24.608 -11.528  1.00 39.62      A
ATOM   2321  OE2  GLU A 298     -6.473  24.342 -13.664  1.00 36.85      A
ATOM   2322  C    GLU A 298     -5.177  27.605 -16.627  1.00 23.08      A
ATOM   2323  O    GLU A 298     -4.175  28.329 -16.679  1.00 21.84      A
ATOM   2324  N    GLN A 299     -5.801  27.151 -17.707  1.00 19.62      A
ATOM   2325  CA   GLN A 299     -5.382  27.476 -19.060  1.00 20.73      A
ATOM   2326  CB   GLN A 299     -5.146  28.988 -19.244  1.00 25.04      A
ATOM   2327  CG   GLN A 299     -6.153  29.921 -18.590  1.00 31.94      A
ATOM   2328  CD   GLN A 299     -5.734  31.391 -18.727  1.00 35.89      A
ATOM   2329  OE1  GLN A 299     -5.505  31.880 -19.840  1.00 38.44      A
ATOM   2330  NE2  GLN A 299     -5.626  32.098 -17.592  1.00 37.47      A
ATOM   2331  C    GLN A 299     -4.089  26.767 -19.419  1.00 18.90      A
ATOM   2332  O    GLN A 299     -3.418  27.164 -20.383  1.00 18.74      A
ATOM   2333  N    GLU A 300     -3.720  25.771 -18.624  1.00 14.58      A
ATOM   2334  CA   GLU A 300     -2.511  24.997 -18.951  1.00 13.30     ,A
ATOM   2335  CB   GLU A 300     -2.035  24.255 -17.708  1.00 14.18     'A
ATOM   2336  CG   GLU A 300     -1.593  25.228 -16.642  1.00 12.48      A
ATOM   2337  CD   GLU A 300     -1.279  24.555 -15.320  1.00 14.90      A
ATOM   2338  OE1  GLU A 300     -1.927  23.543 -14.997  1.00 15.04      A
ATOM   2339  OE2  GLU A 300     -0.394  25.073 -14.582  1.00 17.40      A
ATOM   2340  C    GLU A 300     -2.889  24.054 -20.079  1.00 13.11      A
ATOM   2341  O    GLU A 300     -4.065  23.715 -20.262  1.00 14.26      A
ATOM   2342  N    GLU A 301     -1.899  23.602 -20.856  1.00 12.23      A
ATOM   2343  CA   GLU A 301     -2.215  22.772 -22.001  1.00 13.64      A
ATOM   2344  CB   GLU A 301     -2.406  23.648 -23.246  1.00 17.30      A
ATOM   2345  CG   GLU A 301     -2.865  22.871 -24.488  1.00 22.48      A
ATOM   2346  CD   GLU A 301     -3.254  23.787 -25.635  1.00 27.65      A
ATOM   2347  OE1  GLU A 301     -2.342  24.430 -26.200  1.00 31.10      A
ATOM   2348  OE2  GLU A 301     -4.462  23.877 -25.961  1.00 30.41      A
ATOM   2349  C    GLU A 301     -1.105  21.789 -22.298  1.00 12.28      A
ATOM   2350  O    GLU A 301      0.074  22.112 -22.107  1.00 12.26      A
ATOM   2351  N    ALA A 302     -1.515  20.604 -22.734  1.00 11.02      A
ATOM   2352  CA   ALA A 302     -0.562  19.544 -23.111  1.00 11.63      A
ATOM   2353  CB   ALA A 302     -0.699  18.342 -22.188  1.00 12.84      A
ATOM   2354  C    ALA A 302     -0.834  19.101 -24.550  1.00 13.62      A
ATOM   2355  O    ALA A 302     -1.992  19.077 -25.003  1.00 15.53      A
ATOM   2356  N    GLU A 303      0.223  18.780 -25.301  1.00 10.01      A
ATOM   2357  CA   GLU A 303      0.026  18.255 -26.636  1.00 11.02      A
ATOM   2358  CB   GLU A 303      0.253  19.320 -27.697  1.00 13.49      A
ATOM   2359  CG   GLU A 303      0.127  18.797 -29.115  1.00 15.09      A
ATOM   2360  CD   GLU A 303      0.446  19.851 -30.167  1.00 19.61      A
ATOM   2361  OE1  GLU A 303     -0.479  20.607 -30.584  1.00 20.94      A
ATOM   2362  OE2  GLU A 303      1.628  19.928 -30.579  1.00 18.80      A
ATOM   2363  C    GLU A 303      1.009  17.109 -26.887  1.00 11.44      A
ATOM   2364  O    GLU A 303      2.169  17.226 -26.550  1.00 13.57      A
ATOM   2365  N    GLU A 304      0.513  16.006 -27.427  1.00 10.72      A
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Figure 1 (continued 24)

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ATOM   2366  CA  GLU A 304     1.385  14.866 -27.767  1.00 10.97      A
ATOM   2367  CB  GLU A 304     0.994  13.647 -26.932  1.00 12.53      A
ATOM   2368  CG  GLU A 304     1.248  13.808 -25.483  1.00 12.60      A
ATOM   2369  CD  GLU A 304     2.714  13.563 -25.117  1.00 12.60      A
ATOM   2370  OE1 GLU A 304     3.469  13.052 -25.981  1.00 12.80      A
ATOM   2371  OE2 GLU A 304     3.069  13.867 -23.965  1.00 12.17      A
ATOM   2372  C   GLU A 304     1.147  14.532 -29.244  1.00 12.99      A
ATOM   2373  O   GLU A 304    -0.007  14.450 -29.672  1.00 14.60      A
ATOM   2374  N   ILE A 305     2.205  14.349 -30.033  1.00 11.72      A
ATOM   2375  CA  ILE A 305     1.999  13.953 -31.414  1.00 13.62      A
ATOM   2376  CB  ILE A 305     2.631  14.950 -32.417  1.00 15.28      A
ATOM   2377  CG2 ILE A 305     2.424  14.412 -33.857  1.00 16.72      A
ATOM   2378  CG1 ILE A 305     1.904  16.312 -32.316  1.00 14.51      A
ATOM   2379  CD1 ILE A 305     2.546  17.468 -33.066  1.00 19.83      A
ATOM   2380  C   ILE A 305     2.611  12.557 -31.532  1.00 14.02      A
ATOM   2381  O   ILE A 305     3.727  12.288 -31.012  1.00 13.98      A
ATOM   2382  N   LEU A 306     1.859  11.651 -32.154  1.00 12.94      A
ATOM   2383  CA  LEU A 306     2.313  10.259 -32.344  1.00 14.07      A
ATOM   2384  CB  LEU A 306     1.444   9.265 -31.558  1.00 17.83      A
ATOM   2385  CG  LEU A 306     1.426   9.316 -30.037  1.00 19.01      A
ATOM   2386  CD1 LEU A 306     0.496   8.218 -29.532  1.00 21.97      A
ATOM   2387  CD2 LEU A 306     2.844   9.079 -29.473  1.00 23.23      A
ATOM   2388  C   LEU A 306     2.203   9.831 -33.795  1.00 14.91      A
ATOM   2389  O   LEU A 306     1.284  10.228 -34.487  1.00 14.55      A
ATOM   2390  N   ASP A 307     3.165   9.032 -34.271  1.00 14.49      A
ATOM   2391  CA  ASP A 307     3.013   8.483 -35.615  1.00 16.69      A
ATOM   2392  CB  ASP A 307     4.337   7.966 -36.168  1.00 19.50      A
ATOM   2393  CG  ASP A 307     5.282   9.065 -36.529  1.00 22.90      A
ATOM   2394  OD1 ASP A 307     4.830  10.194 -36.789  1.00 22.13      A
ATOM   2395  OD2 ASP A 307     6.491   8.777 -36.579  1.00 29.27      A
ATOM   2396  C   ASP A 307     2.109   7.266 -35.421  1.00 16.05      A
ATOM   2397  O   ASP A 307     2.294   6.492 -34.470  1.00 16.80      A
ATOM   2398  N   VAL A 308     1.148   7.074 -36.308  1.00 14.24      A
ATOM   2399  CA  VAL A 308     0.244   5.918 -36.228  1.00 14.78      A
ATOM   2400  CB  VAL A 308    -1.128   6.256 -35.539  1.00 14.59      A
ATOM   2401  CG1 VAL A 308    -0.889   6.738 -34.086  1.00 14.50      A
ATOM   2402  CG2 VAL A 308    -1.906   7.299 -36.330  1.00 16.78      A
ATOM   2403  C   VAL A 308    -0.028   5.511 -37.664  1.00 15.25      A
ATOM   2404  O   VAL A 308     0.473   6.156 -38.597  1.00 14.77      A
ATOM   2405  N   THR A 309    -0.820   4.458 -37.849  1.00 15.22      A
ATOM   2406  CA  THR A 309    -1.192   4.055 -39.199  1.00 16.94      A
ATOM   2407  CB  THR A 309    -0.982   2.562 -39.446  1.00 18.38      A
ATOM   2408  OG1 THR A 309     0.392   2.246 -39.265  1.00 20.45      A
ATOM   2409  CG2 THR A 309    -1.399   2.210 -40.906  1.00 21.07      A
ATOM   2410  C   THR A 309    -2.653   4.383 -39.373  1.00 16.41      A
ATOM   2411  O   THR A 309    -3.508   3.790 -38.723  1.00 18.35      A
ATOM   2412  N   TYR A 310    -2.936   5.346 -40.240  1.00 14.86      A
ATOM   2413  CA  TYR A 310    -4.291   5.797 -40.505  1.00 15.78      A
ATOM   2414  CB  TYR A 310    -4.743   6.802 -39.441  1.00 17.41      A
ATOM   2415  CG  TYR A 310    -6.152   7.240 -39.641  1.00 18.61      A
ATOM   2416  CD1 TYR A 310    -7.202   6.359 -39.418  1.00 20.45      A
ATOM   2417  CE1 TYR A 310    -8.519   6.753 -39.640  1.00 22.76      A
ATOM   2418  CD2 TYR A 310    -6.453   8.526 -40.087  1.00 20.08      A
ATOM   2419  CE2 TYR A 310    -7.758   8.926 -40.308  1.00 20.45      A
ATOM   2420  CZ  TYR A 310    -8.787   8.036 -40.087  1.00 22.23      A
ATOM   2421  OH  TYR A 310   -10.077   8.431 -40.323  1.00 23.32      A
ATOM   2422  C   TYR A 310    -4.412   6.478 -41.843  1.00 19.52      A
ATOM   2423  O   TYR A 310    -3.625   7.372 -42.149  1.00 18.32      A
ATOM   2424  N   SER A 311    -5.406   6.070 -42.633  1.00 20.36      A
ATOM   2425  CA  SER A 311    -5.620   6.668 -43.951  1.00 24.14      A
ATOM   2426  CB  SER A 311    -5.341   5.642 -45.027  1.00 24.45      A
ATOM   2427  OG  SER A 311    -6.267   4.577 -44.882  1.00 29.21      A
ATOM   2428  C   SER A 311    -7.028   7.222 -44.203  1.00 26.37      A
ATOM   2429  O   SER A 311    -7.348   7.596 -45.336  1.00 30.35      A
ATOM   2430  N   GLY A 312    -7.880   7.275 -43.196  1.00 28.49      A
ATOM   2431  CA  GLY A 312    -9.217   7.803 -43.441  1.00 28.97      A
ATOM   2432  C   GLY A 312    -9.365   9.320 -43.383  1.00 28.05      A
ATOM   2433  O   GLY A 312    -8.380  10.057 -43.240  1.00 29.05      A
ATOM   2434  N   ALA A 313   -10.607   9.794 -43.303  1.00 27.21      A
ATOM   2435  CA  ALA A 313   -10.876  11.232 -43.199  1.00 24.74      A
ATOM   2436  CB  ALA A 313   -12.346  11.499 -43.370  1.00 26.37      A
ATOM   2437  C   ALA A 313   -10.436  11.749 -41.826  1.00 22.97      A
ATOM   2438  O   ALA A 313   -10.352  10.984 -40.871  1.00 21.96      A
ATOM   2439  N   GLU A 314   -10.168  13.043 -41.720  1.00 20.72      A
ATOM   2440  CA  GLU A 314    -9.756  13.591 -40.439  1.00 18.80      A
ATOM   2441  CB  GLU A 314    -9.055  14.960 -40.587  1.00 17.54      A
ATOM   2442  CG  GLU A 314    -7.815  14.898 -41.505  1.00 16.92      A
ATOM   2443  CD  GLU A 314    -6.990  16.211 -41.564  1.00 13.92      A
ATOM   2444  OE1 GLU A 314    -7.488  17.275 -41.169  1.00 16.98      A
ATOM   2445  OE2 GLU A 314    -5.833  16.145 -42.040  1.00 16.78      A
ATOM   2446  C   GLU A 314   -10.962  13.753 -39.540  1.00 19.37      A
ATOM   2447  O   GLU A 314   -12.103  13.914 -39.997  1.00 19.24      A
ATOM   2448  N   MET A 315   -10.712  13.695 -38.244  1.00 17.56      A
ATOM   2449  CA  MET A 315   -11.773  13.901 -37.273  1.00 18.80      A
ATOM   2450  CB  MET A 315   -12.687  12.671 -37.207  1.00 20.81      A
ATOM   2451  CG  MET A 315   -11.969  11.387 -36.964  1.00 21.30      A
ATOM   2452  SD  MET A 315   -13.164  10.037 -36.647  1.00 27.18      A
ATOM   2453  CE  MET A 315   -13.747  10.557 -35.201  1.00 21.45      A
ATOM   2454  C   MET A 315   -11.181  14.209 -35.907  1.00 18.44      A
ATOM   2455  O   MET A 315   -10.018  13.895 -35.631  1.00 17.20      A
ATOM   2456  N   GLU A 316   -11.973  14.872 -35.075  1.00 16.93      A
ATOM   2457  CA  GLU A 316   -11.563  15.231 -33.736  1.00 18.29      A
ATOM   2458  CB  GLU A 316   -11.582  16.742 -33.551  1.00 21.52      A
ATOM   2459  CG  GLU A 316   -11.083  17.217 -32.220  1.00 27.35      A
ATOM   2460  CD  GLU A 316   -10.835  18.712 -32.316  1.00 32.67      A
ATOM   2461  OE1 GLU A 316   -11.793  19.470 -32.520  1.00 33.72      A
ATOM   2462  OE2 GLU A 316    -9.685  19.135 -31.984  1.00 35.34      A
ATOM   2463  C   GLU A 316   -12.582  14.584 -32.819  1.00 17.89      A
ATOM   2464  O   GLU A 316   -13.801  14.685 -33.042  1.00 20.54      A
ATOM   2465  N   ILE A 317   -12.087  13.908 -31.801  1.00 14.19      A
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Figure 1 (continued 25)

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ATOM   2466   CA   ILE A 317    -12.975   13.213  -30.866   1.00  13.52        A
ATOM   2467   CB   ILE A 317    -13.258   11.774  -31.384   1.00  14.49        A
ATOM   2468   CG2  ILE A 317    -11.953   10.954  -31.387   1.00  12.63        A
ATOM   2469   CG1  ILE A 317    -14.247   11.046  -30.452   1.00  14.36        A
ATOM   2470   CD1  ILE A 317    -14.811    9.786  -31.076   1.00  14.83        A
ATOM   2471   C    ILE A 317    -12.334   13.179  -29.487   1.00  14.51        A
ATOM   2472   O    ILE A 317    -11.106   13.015  -29.353   1.00  13.70        A
ATOM   2473   N    GLY A 318    -13.151   13.355  -28.452   1.00  11.91        A
ATOM   2474   CA   GLY A 318    -12.635   13.353  -27.095   1.00  12.78        A
ATOM   2475   C    GLY A 318    -12.935   12.063  -26.344   1.00  11.89        A
ATOM   2476   O    GLY A 318    -13.880   11.343  -26.682   1.00  13.28        A
ATOM   2477   N    PHE A 319    -12.125   11.754  -25.347   1.00  11.46        A
ATOM   2478   CA   PHE A 319    -12.299   10.573  -24.517   1.00  13.15        A
ATOM   2479   CB   PHE A 319    -11.423    9.386  -25.007   1.00  12.94        A
ATOM   2480   CG   PHE A 319    -11.886    8.802  -26.316   1.00  15.51        A
ATOM   2481   CD1  PHE A 319    -11.104    8.922  -27.448   1.00  17.96        A
ATOM   2482   CD2  PHE A 319    -13.145    8.191  -26.426   1.00  16.52        A
ATOM   2483   CE1  PHE A 319    -11.557    8.453  -28.684   1.00  16.81        A
ATOM   2484   CE2  PHE A 319    -13.594    7.718  -27.660   1.00  17.65        A
ATOM   2485   CZ   PHE A 319    -12.784    7.858  -28.794   1.00  20.90        A
ATOM   2486   C    PHE A 319    -11.891   10.818  -23.103   1.00  12.47        A
ATOM   2487   O    PHE A 319    -10.995   11.607  -22.820   1.00  12.56        A
ATOM   2488   N    ASN A 320    -12.540   10.070  -22.217   1.00  12.28        A
ATOM   2489   CA   ASN A 320    -12.241   10.066  -20.818   1.00  12.72        A
ATOM   2490   CB   ASN A 320    -13.337    9.290  -20.074   1.00  15.27        A
ATOM   2491   CG   ASN A 320    -13.046    9.141  -18.604   1.00  15.22        A
ATOM   2492   OD1  ASN A 320    -12.276    8.268  -18.171   1.00  17.44        A
ATOM   2493   ND2  ASN A 320    -13.668    9.997  -17.806   1.00  18.20        A
ATOM   2494   C    ASN A 320    -10.919    9.318  -20.736   1.00  13.50        A
ATOM   2495   O    ASN A 320    -10.775    8.232  -21.314   1.00  14.56        A
ATOM   2496   N    VAL A 321     -9.948    9.923  -20.051   1.00  13.54        A
ATOM   2497   CA   VAL A 321     -8.627    9.283  -19.905   1.00  15.24        A
ATOM   2498   CB   VAL A 321     -7.661   10.211  -19.117   1.00  14.76        A
ATOM   2499   CG1  VAL A 321     -6.363    9.465  -18.756   1.00  15.84        A
ATOM   2500   CG2  VAL A 321     -7.370   11.417  -19.929   1.00  15.30        A
ATOM   2501   C    VAL A 321     -8.620    7.936  -19.231   1.00  14.40        A
ATOM   2502   O    VAL A 321     -8.011    6.999  -19.749   1.00  16.49        A
ATOM   2503   N    SER A 322     -9.279    7.825  -18.093   1.00  14.64        A
ATOM   2504   CA   SER A 322     -9.247    6.562  -17.370   1.00  16.47        A
ATOM   2505   CB   SER A 322     -9.934    6.699  -15.995   1.00  18.37        A
ATOM   2506   OG   SER A 322    -11.351    6.726  -16.106   1.00  22.86        A
ATOM   2507   C    SER A 322     -9.852    5.443  -18.196   1.00  15.99        A
ATOM   2508   O    SER A 322     -9.372    4.306  -18.142   1.00  14.69        A
ATOM   2509   N    TYR A 323    -10.887    5.743  -18.986   1.00  15.32        A
ATOM   2510   CA   TYR A 323    -11.497    4.659  -19.767   1.00  14.14        A
ATOM   2511   CB   TYR A 323    -12.762    5.104  -20.509   1.00  13.38        A
ATOM   2512   CG   TYR A 323    -13.911    5.510  -19.615   1.00  13.92        A
ATOM   2513   CD1  TYR A 323    -13.925    5.195  -18.261   1.00  15.72        A
ATOM   2514   CE1  TYR A 323    -15.014    5.562  -17.426   1.00  18.29        A
ATOM   2515   CD2  TYR A 323    -14.992    6.184  -20.154   1.00  16.28        A
ATOM   2516   CE2  TYR A 323    -16.080    6.546  -19.337   1.00  16.03        A
ATOM   2517   CZ   TYR A 323    -16.074    6.238  -17.996   1.00  18.77        A
ATOM   2518   OH   TYR A 323    -17.159    6.615  -17.192   1.00  19.53        A
ATOM   2519   C    TYR A 323    -10.522    4.097  -20.798   1.00  13.72        A
ATOM   2520   O    TYR A 323    -10.472    2.871  -20.988   1.00  14.43        A
ATOM   2521   N    VAL A 324     -9.766    4.979  -21.458   1.00  14.57        A
ATOM   2522   CA   VAL A 324     -8.827    4.508  -22.469   1.00  13.06        A
ATOM   2523   CB   VAL A 324     -8.372    5.662  -23.389   1.00  13.33        A
ATOM   2524   CG1  VAL A 324     -7.307    5.165  -24.365   1.00  13.38        A
ATOM   2525   CG2  VAL A 324     -9.556    6.227  -24.142   1.00  13.06        A
ATOM   2526   C    VAL A 324     -7.625    3.863  -21.805   1.00  13.51        A
ATOM   2527   O    VAL A 324     -7.180    2.778  -22.239   1.00  13.91        A
ATOM   3528   N    LEU A 325     -7.103    4.485  -20.749   1.00  13.19        A
ATOM   2529   CA   LEU A 325     -5.958    3.856  -20.062   1.00  12.30        A
ATOM   2530   CB   LEU A 325     -5.421    4.740  -18.922   1.00  14.09        A
ATOM   2531   CG   LEU A 325     -4.756    6.018  -19.451   1.00  15.74        A
ATOM   2532   CD1  LEU A 325     -4.309    6.898  -18.293   1.00  16.69        A
ATOM   2533   CD2  LEU A 325     -3.511    5.670  -20.297   1.00  16.07        A
ATOM   2534   C    LEU A 325     -6.340    2.486  -19.523   1.00  12.94        A
ATOM   2535   O    LEU A 325     -5.530    1.561  -19.557   1.00  13.40        A
ATOM   2536   N    ASP A 326     -7.558    2.333  -18.993   1.00  12.70        A
ATOM   2537   CA   ASP A 326     -7.979    1.036  -18.483   1.00  13.88        A
ATOM   2538   CB   ASP A 326     -9.424    1.066  -17.982   1.00  15.00        A
ATOM   2539   CG   ASP A 326     -9.580    1.726  -16.613   1.00  18.64        A
ATOM   2540   OD1  ASP A 326     -8.568    1.979  -15.900   1.00  17.79        A
ATOM   2541   OD2  ASP A 326    -10.754    2.016  -16.228   1.00  17.43        A
ATOM   2542   C    ASP A 326     -7.882   -0.010  -19.589   1.00  11.78        A
ATOM   2543   O    ASP A 326     -7.433   -1.134  -19.355   1.00  14.48        A
ATOM   2544   N    VAL A 327     -8.349    0.350  -20.785   1.00  12.78        A
ATOM   2545   CA   VAL A 327     -8.317   -0.577  -21.919   1.00  12.19        A
ATOM   2546   CB   VAL A 327     -9.036    0.029  -23.136   1.00  13.17        A
ATOM   2547   CG1  VAL A 327     -8.820   -0.794  -24.388   1.00  13.91        A
ATOM   2548   CG2  VAL A 327    -10.544    0.097  -22.800   1.00  11.68        A
ATOM   2549   C    VAL A 327     -6.889   -0.925  -22.325   1.00  12.85        A
ATOM   2550   O    VAL A 327     -6.582   -2.089  -22.542   1.00  13.03        A
ATOM   2551   N    LEU A 328     -6.037    0.086  -22.418   1.00  13.64        A
ATOM   2552   CA   LEU A 328     -4.646   -0.142  -22.856   1.00  13.56        A
ATOM   2553   CB   LEU A 328     -3.949    1.201  -23.100   1.00  12.03        A
ATOM   2554   CG   LEU A 328     -4.626    2.058  -24.192   1.00  13.75        A
ATOM   2555   CD1  LEU A 328     -3.799    3.306  -24.432   1.00  14.51        A
ATOM   2556   CD2  LEU A 328     -4.758    1.252  -25.503   1.00  15.65        A
ATOM   2557   C    LEU A 328     -3.888   -0.972  -21.825   1.00  16.00        A
ATOM   2558   O    LEU A 328     -2.982   -1.748  -22.174   1.00  17.28        A
ATOM   2559   N    ASN A 329     -4.252   -0.830  -20.557   1.00  14.82        A
ATOM   2560   CA   ASN A 329     -3.639   -1.609  -19.486   1.00  16.78        A
ATOM   2561   CB   ASN A 329     -3.965   -0.957  -18.143   1.00  18.81        A
ATOM   2562   CG   ASN A 329     -3.039    0.182  -17.815   1.00  22.88        A
ATOM   2563   OD1  ASN A 329     -3.410    1.088  -17.067   1.00  27.05        A
ATOM   2564   ND2  ASN A 329     -1.810    0.139  -18.340   1.00  24.22        A
ATOM   2565   C    ASN A 329     -4.112   -3.059  -19.522   1.00  19.68        A
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Figure 1 (continued 26)

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ATOM   2566  O    ASN A 329    -3.353   -3.984 -19.177  1.00 20.96      A
ATOM   2567  N    ALA A 330    -5.347   -3.282 -19.966  1.00 18.19      A
ATOM   2568  CA   ALA A 330    -5.893   -4.635 -20.059  1.00 20.30      A
ATOM   2569  CB   ALA A 330    -7.444   -4.597 -20.070  1.00 20.07      A
ATOM   2570  C    ALA A 330    -5.385   -5.363 -21.304  1.00 20.84      A
ATOM   2571  O    ALA A 330    -5.261   -6.601 -21.312  1.00 21.96      A
ATOM   2572  N    LEU A 331    -5.092   -4.614 -22.365  1.00 20.51      A
ATOM   2573  CA   LEU A 331    -4.607   -5.238 -23.606  1.00 22.56      A
ATOM   2574  CB   LEU A 331    -4.857   -4.311 -24.807  1.00 19.58      A
ATOM   2575  CG   LEU A 331    -6.319   -4.242 -25.284  1.00 20.93      A
ATOM   2576  CD1  LEU A 331    -6.493   -3.076 -26.290  1.00 20.46      A
ATOM   2577  CD2  LEU A 331    -6.749   -5.570 -25.905  1.00 19.08      A
ATOM   2578  C    LEU A 331    -3.127   -5.621 -23.508  1.00 25.46      A
ATOM   2579  O    LEU A 331    -2.742   -6.688 -23.998  1.00 27.06      A
ATOM   2580  N    LYS A 332    -2.313   -4.753 -22.903  1.00 26.68      A
ATOM   2581  CA   LYS A 332    -0.877   -5.002 -22.724  1.00 28.23      A
ATOM   2582  CB   LYS A 332    -0.651   -5.661 -21.356  1.00 29.27      A
ATOM   2583  CG   LYS A 332    -1.401   -6.966 -21.184  1.00 29.90      A
ATOM   2584  CD   LYS A 332    -1.468   -7.412 -19.728  1.00 32.09      A
ATOM   2585  CE   LYS A 332    -2.173   -8.745 -19.658  1.00 32.35      A
ATOM   2586  NZ   LYS A 332    -2.345   -9.225 -18.268  1.00 35.40      A
ATOM   2587  C    LYS A 332    -0.266   -5.853 -23.855  1.00 27.53      A
ATOM   2588  O    LYS A 332     0.361   -6.884 -23.618  1.00 31.18      A
ATOM   2589  N    CYS A 333    -0.484   -5.404 -25.087  1.00 25.22      A
ATOM   2590  CA   CYS A 333     0.010   -6.074 -26.301  1.00 21.25      A
ATOM   2591  CB   CYS A 333    -1.158   -6.522 -27.166  1.00 19.35      A
ATOM   2592  SG   CYS A 333    -2.257   -5.131 -27.559  1.00 20.24      A
ATOM   2593  C    CYS A 333     0.878   -5.087 -27.069  1.00 20.62      A
ATOM   2594  O    CYS A 333     1.047   -3.966 -26.640  1.00 20.60      A
ATOM   2595  N    GLU A 334     1.422   -5.490 -28.218  1.00 19.42      A
ATOM   2596  CA   GLU A 334     2.317   -4.604 -28.956  1.00 19.82      A
ATOM   2597  CB   GLU A 334     3.102   -5.421 -29.998  1.00 21.89      A
ATOM   2598  CG   GLU A 334     4.169   -4.662 -30.765  1.00 27.12      A
ATOM   2599  CD   GLU A 334     5.320   -4.181 -29.882  1.00 29.45      A
ATOM   2600  OE1  GLU A 334     5.657   -4.863 -28.890  1.00 32.60      A
ATOM   2601  OE2  GLU A 334     5.902   -3.121 -30.198  1.00 32.88      A
ATOM   2602  C    GLU A 334     1.625   -3.429 -29.636  1.00 16.58      A
ATOM   2603  O    GLU A 334     2.060   -2.292 -29.474  1.00 16.78      A
ATOM   2604  N    ASN A 335     0.576   -3.704 -30.402  1.00 16.51      A
ATOM   2605  CA   ASN A 335    -0.146   -2.651 -31.136  1.00 15.36      A
ATOM   2606  CB   ASN A 335     0.089   -2.780 -32.566  1.00 18.00      A
ATOM   2607  CG   ASN A 335     1.546   -2.690 -33.022  1.00 20.47      A
ATOM   2608  OD1  ASN A 335     2.162   -3.672 -33.464  1.00 25.38      A
ATOM   2609  ND2  ASN A 335     2.103   -1.518 -32.867  1.00 18.14      A
ATOM   2610  C    ASN A 335    -1.646   -2.792 -30.914  1.00 16.50      A
ATOM   2611  O    ASN A 335    -2.167   -3.914 -30.726  1.00 16.59      A
ATOM   2612  N    VAL A 336    -2.327   -1.661 -30.918  1.00 16.20      A
ATOM   2613  CA   VAL A 336    -3.764   -1.655 -30.767  1.00 14.76      A
ATOM   2614  CB   VAL A 336    -4.247   -0.853 -29.501  1.00 16.01      A
ATOM   2615  CG1  VAL A 336    -3.681   -1.469 -28.239  1.00 19.32      A
ATOM   2616  CG2  VAL A 336    -3.854    0.619 -29.614  1.00 18.64      A
ATOM   2617  C    VAL A 336    -4.390   -1.040 -31.993  1.00 16.20      A
ATOM   2618  O    VAL A 336    -3.766   -0.257 -32.719  1.00 15.92      A
ATOM   2619  N    ARG A 337    -5.631   -1.422 -32.238  1.00 16.08      A
ATOM   2620  CA   ARG A 337    -6.391   -0.860 -33.330  1.00 17.59      A
ATOM   2621  CB   ARG A 337    -6.879   -1.961 -34.281  1.00 20.37      A
ATOM   2622  CG   ARG A 337    -7.779   -1.445 -35.423  1.00 24.09      A
ATOM   2623  CD   ARG A 337    -8.161   -2.499 -36.481  1.00 26.96      A
ATOM   2624  NE   ARG A 337    -6.983   -3.165 -37.020  1.00 29.58      A
ATOM   2625  CZ   ARG A 337    -6.568   -4.369 -36.628  1.00 30.93      A
ATOM   2626  NH1  ARG A 337    -7.254   -5.040 -35.706  1.00 33.27      A
ATOM   2627  NH2  ARG A 337    -5.446   -4.880 -37.124  1.00 31.58      A
ATOM   2628  C    ARG A 337    -7.602   -0.160 -32.741  1.00 17.83      A
ATOM   2629  O    ARG A 337    -8.342   -0.739 -31.919  1.00 17.99      A
ATOM   2630  N    MET A 338    -7.803    1.092 -33.154  1.00 16.35      A
ATOM   2631  CA   MET A 338    -8.976    1.881 -32.731  1.00 17.54      A
ATOM   2632  CB   MET A 338    -8.561    3.298 -32.322  1.00 19.03      A
ATOM   2633  CG   MET A 338    -7.696    3.343 -31.067  1.00 22.98      A
ATOM   2634  SD   MET A 338    -7.251    5.013 -30.485  1.00 28.14      A
ATOM   2635  CE   MET A 338    -8.672    5.347 -29.411  1.00 24.78      A
ATOM   2636  C    MET A 338    -9.867    1.943 -33.963  1.00 17.28      A
ATOM   2637  O    MET A 338    -9.398    2.321 -35.033  1.00 18.78      A
ATOM   2638  N    MET A 339   -11.144    1.591 -33.825  1.00 17.39      A
ATOM   2639  CA   MET A 339   -12.064    1.582 -34.955  1.00 17.39      A
ATOM   2640  CB   MET A 339   -12.686    0.180 -35.053  1.00 20.98      A
ATOM   2641  CG   MET A 339   -11.628   -0.888 -34.852  1.00 25.07      A
ATOM   2642  SD   MET A 339   -12.307   -2.536 -34.442  1.00 30.90      A
ATOM   2643  CE   MET A 339   -12.758   -2.891 -36.141  1.00 27.62      A
ATOM   2644  C    MET A 339   -13.075   -2.454 -34.673  1.00 18.45      A
ATOM   2645  O    MET A 339   -13.868   -2.596 -33.729  1.00 17.17      A
ATOM   2646  N    LEU A 340   -13.009    3.728 -35.490  1.00 17.41      A
ATOM   2647  CA   LEU A 340   -13.853    4.898 -35.313  1.00 19.07      A
ATOM   2648  CB   LEU A 340   -12.974    6.150 -35.330  1.00 21.15      A
ATOM   2649  CG   LEU A 340   -11.856    6.140 -34.291  1.00 22.56      A
ATOM   2650  CD1  LEU A 340   -10.597    6.765 -34.885  1.00 27.71      A
ATOM   2651  CD2  LEU A 340   -12.321    6.886 -33.043  1.00 24.99      A
ATOM   2652  C    LEU A 340   -14.892    5.036 -36.396  1.00 20.06      A
ATOM   2653  O    LEU A 340   -14.739    4.483 -37.481  1.00 20.26      A
ATOM   2654  N    THR A 341   -15.941    5.783 -36.086  1.00 22.17      A
ATOM   2655  CA   THR A 341   -17.029    6.020 -37.026  1.00 25.08      A
ATOM   2656  CB   THR A 341   -18.360    5.576 -36.433  1.00 26.10      A
ATOM   2657  OG1  THR A 341   -18.287    4.178 -36.133  1.00 25.61      A
ATOM   2658  CG2  THR A 341   -19.487    5.811 -37.438  1.00 26.42      A
ATOM   2659  C    THR A 341   -17.084    7.509 -37.328  1.00 25.45      A
ATOM   2660  O    THR A 341   -16.921    7.922 -38.481  1.00 27.99      A
ATOM   2661  N    ASP A 342   -17.320    8.298 -36.284  1.00 25.19      A
ATOM   2662  CA   ASP A 342   -17.367    9.757 -36.381  1.00 24.72      A
ATOM   2663  CB   ASP A 342   -18.690   10.235 -37.008  1.00 25.68      A
ATOM   2664  CG   ASP A 342   -19.905    9.816 -36.214  1.00 27.08      A
ATOM   2665  OD1  ASP A 342   -19.828    9.819 -34.967  1.00 25.89      A
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Figure 1 (continued 27)

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ATOM   2666  OD2 ASP A 342    -20.947    9.513  -36.855  1.00 30.26      A
ATOM   2667  C   ASP A 342    -17.137   10.406  -35.019  1.00 23.68      A
ATOM   2668  O   ASP A 342    -16.889    9.725  -34.014  1.00 21.46      A
ATOM   2669  N   SER A 343    -17.216   11.729  -34.969  1.00 23.14      A
ATOM   2670  CA  SER A 343    -16.929   12.436  -33.744  1.00 24.43      A
ATOM   2671  CB  SER A 343    -16.755   13.936  -34.034  1.00 26.47      A
ATOM   2672  OG  SER A 343    -17.994   14.549  -34.368  1.00 29.79      A
ATOM   2673  C   SER A 343    -17.905   12.249  -32.602  1.00 24.03      A
ATOM   2674  O   SER A 343    -17.567   12.520  -31.457  1.00 24.30      A
ATOM   2675  N   VAL A 344    -19.109   11.758  -32.884  1.00 23.83      A
ATOM   2676  CA  VAL A 344    -20.078   11.630  -31.809  1.00 23.12      A
ATOM   2677  CB  VAL A 344    -21.357   12.448  -32.132  1.00 24.91      A
ATOM   2678  CG1 VAL A 344    -21.003   13.909  -32.356  1.00 25.01      A
ATOM   2679  CG2 VAL A 344    -22.011   11.888  -33.359  1.00 23.59      A
ATOM   2680  C   VAL A 344    -20.487   10.192  -31.504  1.00 23.42      A
ATOM   2681  O   VAL A 344    -21.458    9.951  -30.788  1.00 25.49      A
ATOM   2682  N   SER A 345    -19.731    9.244  -32.026  1.00 21.89      A
ATOM   2683  CA  SER A 345    -20.013    7.829  -31.834  1.00 21.04      A
ATOM   2684  CB  SER A 345    -20.163    7.177  -33.197  1.00 22.41      A
ATOM   2685  OG  SER A 345    -21.229    7.826  -33.898  1.00 25.59      A
ATOM   2686  C   SER A 345    -18.903    7.139  -31.038  1.00 20.75      A
ATOM   2687  O   SER A 345    -17.768    7.582  -31.036  1.00 20.76      A
ATOM   2688  N   SER A 346    -19.241    6.045  -30.367  1.00 18.72      A
ATOM   2689  CA  SER A 346    -18.246    5.326  -29.580  1.00 17.41      A
ATOM   2690  CB  SER A 346    -18.942    4.243  -28.764  1.00 18.74      A
ATOM   2691  OG  SER A 346    -19.913    4.838  -27.930  1.00 22.66      A
ATOM   2692  C   SER A 346    -17.184    4.697  -30.466  1.00 17.40      A
ATOM   2693  O   SER A 346    -17.398    4.490  -31.656  1.00 21.59      A
ATOM   2694  N   VAL A 347    -16.045    4.390  -29.869  1.00 16.03      A
ATOM   2695  CA  VAL A 347    -14.916    3.754  -30.558  1.00 15.59      A
ATOM   2696  CB  VAL A 347    -13.561    4.492  -30.225  1.00 16.49      A
ATOM   2697  CG1 VAL A 347    -13.206    4.415  -28.731  1.00 17.48      A
ATOM   2698  CG2 VAL A 347    -12.426    3.924  -31.045  1.00 19.46      A
ATOM   2699  C   VAL A 347    -14.809    2.305  -30.088  1.00 14.00      A
ATOM   2700  O   VAL A 347    -15.213    2.005  -28.974  1.00 15.79      A
ATOM   2701  N   GLN A 348    -14.340    1.420  -30.957  1.00 13.62      A
ATOM   2702  CA  GLN A 348    -14.081    0.025  -30.547  1.00 12.23      A
ATOM   2703  CB  GLN A 348    -14.702   -0.983  -31.533  1.00 13.64      A
ATOM   2704  CG  GLN A 348    -14.416   -2.454  -31.162  1.00 15.65      A
ATOM   2705  CD  GLN A 348    -15.268   -3.431  -31.957  1.00 16.97      A
ATOM   2706  OE1 GLN A 348    -14.825   -4.545  -32.272  1.00 22.42      A
ATOM   2707  NE2 GLN A 348    -16.499   -3.035  -32.262  1.00 16.85      A
ATOM   2708  C   GLN A 348    -12.548   -0.121  -30.580  1.00 13.90      A
ATOM   2709  O   GLN A 348    -11.909    0.275  -31.563  1.00 13.82      A
ATOM   2710  N   ILE A 349    -11.971   -0.681  -29.513  1.00 12.76      A
ATOM   2711  CA  ILE A 349    -10.516   -0.865  -29.425  1.00 12.30      A
ATOM   2712  CB  ILE A 349     -9.967   -0.071  -28.210  1.00 14.15      A
ATOM   2713  CG2 ILE A 349     -8.434   -0.148  -28.138  1.00 14.43      A
ATOM   2714  CG1 ILE A 349    -10.359    1.398  -28.357  1.00 13.90      A
ATOM   2715  CD1 ILE A 349     -9.959    2.196  -27.088  1.00 14.25      A
ATOM   2716  C   ILE A 349    -10.232   -2.339  -29.247  1.00 14.06      A
ATOM   2717  O   ILE A 349    -10.933   -3.012  -28.480  1.00 14.91      A
ATOM   2718  N   GLU A 350     -9.195   -2.824  -29.938  1.00 14.83      A
ATOM   2719  CA  GLU A 350     -8.765   -4.231  -29.850  1.00 15.53      A
ATOM   2720  CB  GLU A 350     -9.357   -5.077  -30.975  1.00 17.90      A
ATOM   2721  CG  GLU A 350    -10.870   -5.018  -31.138  1.00 19.30      A
ATOM   2722  CD  GLU A 350    -11.361   -5.919  -32.260  1.00 24.15      A
ATOM   2723  OE1 GLU A 350    -10.523   -6.447  -33.034  1.00 25.09      A
ATOM   2724  OE2 GLU A 350    -12.589   -6.095  -32.374  1.00 23.78      A
ATOM   2725  C   GLU A 350     -7.247   -4.312  -30.037  1.00 15.60      A
ATOM   2726  O   GLU A 350     -6.600   -3.359  -30.479  1.00 15.29      A
ATOM   2727  N   ASP A 351     -6.693   -5.471  -29.693  1.00 16.12      A
ATOM   2728  CA  ASP A 351     -5.276   -5.765  -29.898  1.00 15.76      A
ATOM   2729  CB  ASP A 351     -4.976   -7.144  -29.283  1.00 15.10      A
ATOM   2730  CG  ASP A 351     -3.542   -7.604  -29.489  1.00 17.20      A
ATOM   2731  OD1 ASP A 351     -2.865   -7.057  -30.377  1.00 17.43      A
ATOM   2732  OD2 ASP A 351     -3.085   -8.526  -28.744  1.00 18.87      A
ATOM   2733  C   ASP A 351     -5.253   -5.849  -31.438  1.00 15.75      A
ATOM   2734  O   ASP A 351     -6.140   -6.458  -32.049  1.00 16.51      A
ATOM   2735  N   ALA A 352     -4.278   -5.224  -32.096  1.00 16.21      A
ATOM   2736  CA  ALA A 352     -4.269   -5.276  -33.558  1.00 18.09      A
ATOM   2737  CB  ALA A 352     -3.158   -4.347  -34.121  1.00 18.36      A
ATOM   2738  C   ALA A 352     -4.046   -6.711  -34.030  1.00 18.81      A
ATOM   2739  O   ALA A 352     -4.396   -7.044  -35.158  1.00 21.06      A
ATOM   2740  N   ALA A 353     -3.496   -7.552  -33.157  1.00 19.56      A
ATOM   2741  CA  ALA A 353     -3.194   -8.946  -33.502  1.00 20.21      A
ATOM   2742  CB  ALA A 353     -1.792   -9.285  -33.026  1.00 20.26      A
ATOM   2743  C   ALA A 353     -4.167  -10.006  -32.977  1.00 21.68      A
ATOM   2744  O   ALA A 353     -3.901  -11.201  -33.108  1.00 23.17      A
ATOM   2745  N   SER A 354     -5.281   -9.598  -32.382  1.00 20.83      A
ATOM   2746  CA  SER A 354     -6.225  -10.577  -31.843  1.00 19.77      A
ATOM   2747  CB  SER A 354     -5.780  -11.029  -30.468  1.00 20.42      A
ATOM   2748  OG  SER A 354     -6.738  -11.943  -29.917  1.00 22.32      A
ATOM   2749  C   SER A 354     -7.597   -9.986  -31.687  1.00 20.59      A
ATOM   2750  O   SER A 354     -7.720   -8.890  -31.151  1.00 19.79      A
ATOM   2751  N   GLN A 355     -8.618  -10.720  -32.129  1.00 20.97      A
ATOM   2752  CA  GLN A 355     -9.990  -10.266  -32.014  1.00 22.47      A
ATOM   2753  CB  GLN A 355    -10.786  -10.602  -33.278  1.00 26.42      A
ATOM   2754  CG  GLN A 355    -10.487   -9.680  -34.457  1.00 29.56      A
ATOM   2755  CD  GLN A 355    -11.532   -9.777  -35.552  1.00 32.83      A
ATOM   2756  OE1 GLN A 355    -12.725   -9.567  -35.307  1.00 34.38      A
ATOM   2757  NE2 GLN A 355    -11.088  -10.083  -36.773  1.00 33.96      A
ATOM   2758  C   GLN A 355    -10.664  -10.924  -30.809  1.00 20.74      A
ATOM   2759  O   GLN A 355    -11.869  -10.815  -30.648  1.00 23.27      A
ATOM   2760  N   SER A 356     -9.887  -11.573  -29.956  1.00 18.84      A
ATOM   2761  CA  SER A 356    -10.456  -12.239  -28.769  1.00 19.15      A
ATOM   2762  CB  SER A 356     -9.386  -13.050  -28.027  1.00 19.93      A
ATOM   2763  OG  SER A 356     -8.338  -12.230  -27.573  1.00 26.23      A
ATOM   2764  C   SER A 356    -11.136  -11.293  -27.793  1.00 17.16      A
ATOM   2765  C   SER A 356    -12.118  -11.664  -27.158  1.00 17.71      A
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Figure 1 (continued 28)

ATOM	2766	N	ALA A 357	-10.623	-10.084	-27.649	1.00	16.33	A
ATOM	2767	CA	ALA A 357	-11.258	-9.113	-26.750	1.00	16.01	A
ATOM	2768	CB	ALA A 357	-10.362	-8.779	-25.603	1.00	17.39	A
ATOM	2769	C	ALA A 357	-11.590	-7.841	-27.524	1.00	15.77	A
ATOM	2770	O	ALA A 357	-10.883	-7.481	-28.477	1.00	18.23	A
ATOM	2771	N	ALA A 358	-12.673	-7.180	-27.129	1.00	15.41	A
ATOM	2772	CA	ALA A 358	-13.047	-5.907	-27.761	1.00	12.42	A
ATOM	2773	CB	ALA A 358	-14.140	-6.118	-28.811	1.00	14.36	A
ATOM	2774	C	ALA A 358	-13.535	-4.944	-26.677	1.00	13.39	A
ATOM	2775	O	ALA A 358	-14.168	-5.354	-25.689	1.00	13.08	A
ATOM	2776	N	TYR A 359	-13.250	-3.662	-26.853	1.00	11.92	A
ATOM	2777	CA	TYR A 359	-13.638	-2.664	-25.873	1.00	12.31	A
ATOM	2778	CB	TYR A 359	-12.385	-2.123	-25.143	1.00	12.39	A
ATOM	2779	CG	TYR A 359	-11.605	-3.220	-24.463	1.00	12.04	A
ATOM	2780	CD1	TYR A 359	-11.895	-3.596	-23.151	1.00	11.11	A
ATOM	2781	CE1	TYR A 359	-11.257	-4.683	-22.558	1.00	12.06	A
ATOM	2782	CD2	TYR A 359	-10.643	-3.958	-25.175	1.00	12.43	A
ATOM	2783	CE2	TYR A 359	-10.014	-5.054	-24.588	1.00	12.80	A
ATOM	2784	CZ	TYR A 359	-10.328	-5.396	-23.286	1.00	13.52	A
ATOM	2785	OH	TYR A 359	-9.665	-6.468	-22.703	1.00	14.61	A
ATOM	2786	C	TYR A 359	-14.380	-1.543	-26.564	1.00	12.62	A
ATOM	2787	O	TYR A 359	-14.014	-1.160	-27.671	1.00	13.90	A
ATOM	2788	N	VAL A 360	-15.470	-1.072	-25.961	1.00	12.93	A
ATOM	2789	CA	VAL A 360	-16.245	0.015	-26.567	1.00	14.00	A
ATOM	2790	CB	VAL A 360	-17.670	-0.433	-26.861	1.00	12.46	A
ATOM	2791	CG1	VAL A 360	-18.476	0.737	-27.477	1.00	15.11	A
ATOM	2792	CG2	VAL A 360	-17.624	-1.638	-27.791	1.00	14.89	A
ATOM	2793	C	VAL A 360	-16.255	1.158	-25.586	1.00	13.57	A
ATOM	2794	O	VAL A 360	-16.573	0.967	-24.419	1.00	12.80	A
ATOM	2795	N	VAL A 361	-15.883	2.359	-26.044	1.00	13.11	A
ATOM	2796	CA	VAL A 361	-15.821	3.496	-25.157	1.00	14.02	A
ATOM	2797	CB	VAL A 361	-14.346	3.931	-24.924	1.00	13.31	A
ATOM	2798	CG1	VAL A 361	-14.272	5.047	-23.911	1.00	14.14	A
ATOM	2799	CG2	VAL A 361	-13.542	2.718	-24.402	1.00	14.27	A
ATOM	2800	C	VAL A 361	-16.566	4.648	-25.785	1.00	13.41	A
ATOM	2801	O	VAL A 361	-16.339	4.947	-26.948	1.00	13.82	A
ATOM	2802	N	MET A 362	-17.494	5.247	-25.043	1.00	14.34	A
ATOM	2803	CA	MET A 362	-18.208	6.383	-25.612	1.00	15.43	A
ATOM	2804	CB	MET A 362	-19.406	6.802	-24.729	1.00	17.04	A
ATOM	2805	CG	MET A 362	-20.532	5.811	-24.542	1.00	24.10	A
ATOM	2806	SD	MET A 362	-21.744	6.650	-23.450	1.00	30.22	A
ATOM	2807	CE	MET A 362	-20.595	7.445	-22.182	1.00	27.70	A
ATOM	2808	C	MET A 362	-17.290	7.592	-25.674	1.00	16.05	A
ATOM	2809	O	MET A 362	-16.327	7.689	-24.949	1.00	16.00	A
ATOM	2810	N	PRO A 363	-17.602	8.535	-26.550	1.00	16.34	A
ATOM	2811	CD	PRO A 363	-18.565	8.438	-27.661	1.00	19.07	A
ATOM	2812	CA	PRO A 363	-16.771	9.736	-26.643	1.00	17.39	A
ATOM	2813	CB	PRO A 363	-17.127	10.292	-28.017	1.00	20.19	A
ATOM	2814	CG	PRO A 363	-18.547	9.841	-28.237	1.00	20.14	A
ATOM	2815	C	PRO A 363	-17.113	10.686	-25.490	1.00	18.96	A
ATOM	2816	O	PRO A 363	-18.201	10.583	-24.888	1.00	19.41	A
ATOM	2817	N	MET A 364	-16.172	11.557	-25.138	1.00	17.22	A
ATOM	2818	CA	MET A 364	-16.369	12.584	-24.095	1.00	16.88	A
ATOM	2819	CB	MET A 364	-15.308	12.451	-22.998	1.00	18.63	A
ATOM	2820	CG	MET A 364	-15.448	13.444	-21.856	1.00	19.86	A
ATOM	2821	SD	MET A 364	-14.143	13.161	-20.684	1.00	20.18	A
ATOM	2822	CE	MET A 364	-14.902	12.079	-19.580	1.00	21.47	A
ATOM	2823	C	MET A 364	-16.309	13.976	-24.722	1.00	19.03	A
ATOM	2824	O	MET A 364	-15.394	14.297	-25.489	1.00	19.46	A
ATOM	2825	N	ARG A 365	-17.297	14.828	-24.430	1.00	18.40	A
ATOM	2826	CA	ARG A 365	-17.304	16.180	-24.984	1.00	21.57	A
ATOM	2827	CB	ARG A 365	-18.723	16.759	-24.976	1.00	23.93	A
ATOM	2828	CG	ARG A 365	-19.660	16.122	-25.961	1.00	30.14	A
ATOM	2829	CD	ARG A 365	-19.240	16.437	-27.376	1.00	35.93	A
ATOM	2830	NE	ARG A 365	-20.353	16.314	-28.317	1.00	41.53	A
ATOM	2831	CZ	ARG A 365	-20.214	16.355	-29.639	1.00	43.21	A
ATOM	2832	NH1	ARG A 365	-19.009	16.526	-30.174	1.00	43.54	A
ATOM	2833	NH2	ARG A 365	-21.281	16.282	-30.426	1.00	44.53	A
ATOM	2834	C	ARG A 365	-16.402	17.079	-24.164	1.00	20.31	A
ATOM	2835	O	ARG A 365	-16.487	17.099	-22.932	1.00	19.99	A
ATOM	2836	N	LEU A 366	-15.549	17.842	-24.850	1.00	19.74	A
ATOM	2837	CA	LEU A 366	-14.637	18.744	-24.152	1.00	21.42	A
ATOM	2838	CB	LEU A 366	-13.205	18.186	-24.236	1.00	21.30	A
ATOM	2839	CG	LEU A 366	-12.987	16.831	-23.568	1.00	22.44	A
ATOM	2840	CD1	LEU A 366	-11.670	16.240	-24.049	1.00	22.25	A
ATOM	2841	CD2	LEU A 366	-12.952	16.997	-22.073	1.00	21.14	A
ATOM	2842	C	LEU A 366	-14.675	20.182	-24.703	1.00	23.50	A
ATOM	2843	O	LEU A 366	-13.631	20.879	-24.600	1.00	24.15	A
ATOM	2844	OXT	LEU A 366	-15.757	20.610	-25.202	1.00	25.87	A
ATOM	2845	CB	MET B 1	14.354	31.226	-16.722	1.00	14.72	B
ATOM	2846	CG	MET B 1	14.917	30.008	-15.980	1.00	13.54	B
ATOM	2847	SD	MET B 1	13.753	29.266	-14.804	1.00	17.51	B
ATOM	2848	CE	MET B 1	12.697	28.387	-15.952	1.00	16.34	B
ATOM	2849	C	MET B 1	14.966	30.414	-18.998	1.00	14.66	B
ATOM	2850	O	MET B 1	13.867	30.217	-19.542	1.00	16.39	B
ATOM	2851	N	MET B 1	14.668	32.827	-18.638	1.00	16.03	B
ATOM	2852	CA	MET B 1	15.135	31.538	-18.017	1.00	13.94	B
ATOM	2853	N	LYS B 2	16.047	29.666	-19.238	1.00	14.97	B
ATOM	2854	CA	LYS B 2	16.015	28.554	-20.195	1.00	15.37	B
ATOM	2855	CB	LYS B 2	16.413	29.068	-21.575	1.00	17.84	B
ATOM	2856	CG	LYS B 2	16.273	28.083	-22.709	1.00	23.16	B
ATOM	2857	CD	LYS B 2	16.371	28.841	-24.054	1.00	27.33	B
ATOM	2858	CE	LYS B 2	15.972	27.950	-25.222	1.00	30.66	B
ATOM	2859	NZ	LYS B 2	16.920	26.805	-25.375	1.00	31.91	B
ATOM	2860	C	LYS B 2	17.004	27.477	-19.805	1.00	16.00	B
ATOM	2861	O	LYS B 2	18.106	27.776	-19.356	1.00	14.43	B
ATOM	2862	N	PHE B 3	16.592	26.224	-19.918	1.00	12.71	B
ATOM	2863	CA	PHE B 3	17.524	25.132	-19.669	1.00	13.78	B
ATOM	2864	CB	PHE B 3	17.744	24.912	-18.154	1.00	12.36	B
ATOM	2865	CG	PHE B 3	16.521	24.464	-17.403	1.00	11.46	B

Figure 1 (continued 29)

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ATOM   2866  CD1 PHE B   3    15.726  25.391 -16.719  1.00 12.95       B
ATOM   2867  CD2 PHE B   3    16.192  23.108 -17.354  1.00 11.17       B
ATOM   2868  CE1 PHE B   3    14.607  24.944 -15.988  1.00 13.10       B
ATOM   2869  CE2 PHE B   3    15.088  22.664 -16.639  1.00 13.73       B
ATOM   2870  CZ  PHE B   3    14.300  23.598 -15.956  1.00 11.90       B
ATOM   2871  C   PHE B   3    17.047  23.862 -20.358  1.00 12.91       B
ATOM   2872  O   PHE B   3    15.870  23.705 -20.657  1.00 14.61       B
ATOM   2873  N   THR B   4    17.981  22.983 -20.677  1.00 12.44       B
ATOM   2874  CA  THR B   4    17.647  21.694 -21.264  1.00 12.80       B
ATOM   2875  CB  THR B   4    18.054  21.570 -22.727  1.00 14.32       B
ATOM   2876  OG1 THR B   4    17.465  22.636 -23.492  1.00 17.57       B
ATOM   2877  CG2 THR B   4    17.564  20.235 -23.258  1.00 15.46       B
ATOM   2878  C   THR B   4    18.437  20.668 -20.440  1.00 14.04       B
ATOM   2879  O   THR B   4    19.658  20.774 -20.291  1.00 14.28       B
ATOM   2880  N   VAL B   5    17.740  19.692 -19.870  1.00 14.07       B
ATOM   2881  CA  VAL B   5    18.377  18.702 -19.003  1.00 14.50       B
ATOM   2882  CB  VAL B   5    18.137  19.055 -17.497  1.00 14.63       B
ATOM   2883  CG1 VAL B   5    18.774  17.995 -16.572  1.00 19.00       B
ATOM   2884  CG2 VAL B   5    18.711  20.379 -17.153  1.00 19.65       B
ATOM   2885  C   VAL B   5    17.841  17.296 -19.293  1.00 16.13       B
ATOM   2886  O   VAL B   5    16.685  17.117 -19.675  1.00 16.46       B
ATOM   2887  N   GLU B   6    18.694  16.294 -19.151  1.00 15.26       B
ATOM   2888  CA  GLU B   6    18.295  14.932 -19.348  1.00 14.93       B
ATOM   2889  CB  GLU B   6    19.563  14.057 -19.314  1.00 17.40       B
ATOM   2890  CG  GLU B   6    19.320  12.568 -19.294  1.00 24.92       B
ATOM   2891  CD  GLU B   6    20.397  11.849 -18.509  1.00 30.16       B
ATOM   2892  OE1 GLU B   6    21.409  11.429 -19.117  1.00 31.47       B
ATOM   2893  OE2 GLU B   6    20.235  11.721 -17.269  1.00 30.79       B
ATOM   2894  C   GLU B   6    17.304  14.577 -18.204  1.00 14.96       B
ATOM   2895  O   GLU B   6    17.478  14.983 -17.044  1.00 13.59       B
ATOM   2896  N   ARG B   7    16.268  13.831 -18.547  1.00 13.17       B
ATOM   2897  CA  ARG B   7    15.235  13.435 -17.595  1.00 13.08       B
ATOM   2898  CB  ARG B   7    14.341  12.368 -18.216  1.00 12.64       B
ATOM   2899  CG  ARG B   7    13.332  11.764 -17.240  1.00 11.85       B
ATOM   2900  CD  ARG B   7    12.547  10.721 -17.988  1.00 14.66       B
ATOM   2901  NE  ARG B   7    11.561  10.026 -17.142  1.00 13.57       B
ATOM   2902  CZ  ARG B   7    11.809   8.942 -16.404  1.00 17.64       B
ATOM   2903  NH1 ARG B   7    13.015   8.381 -16.365  1.00 17.50       B
ATOM   2904  NH2 ARG B   7    10.839   8.391 -15.706  1.00 15.79       B
ATOM   2905  C   ARG B   7    15.748  12.932 -16.243  1.00 14.94       B
ATOM   2906  O   ARG B   7    15.326  13.421 -15.202  1.00 13.48       B
ATOM   2907  N   GLU B   8    16.679  11.981 -16.256  1.00 15.15       B
ATOM   2908  CA  GLU B   8    17.145  11.434 -14.973  1.00 18.15       B
ATOM   2909  CB  GLU B   8    17.861  10.104 -15.238  1.00 18.04       B
ATOM   2910  CG  GLU B   8    16.929   9.035 -15.849  1.00 19.35       B
ATOM   2911  CD  GLU B   8    16.576   9.297 -17.297  1.00 17.91       B
ATOM   2912  OE1 GLU B   8    17.433   9.801 -18.024  1.00 19.66       B
ATOM   2913  OE2 GLU B   8    15.460   8.978 -17.745  1.00 18.19       B
ATOM   2914  C   GLU B   8    17.988  12.368 -14.103  1.00 20.48       B
ATOM   2915  O   GLU B   8    18.056  12.219 -12.878  1.00 19.63       B
ATOM   2916  N   HIS B   9    18.613  13.364 -14.728  1.00 21.28       B
ATOM   2917  CA  HIS B   9    19.426  14.333 -14.008  1.00 23.49       B
ATOM   2918  CB  HIS B   9    20.297  15.041 -15.071  1.00 25.02       B
ATOM   2919  CG  HIS B   9    21.522  15.711 -14.538  1.00 25.42       B
ATOM   2920  CD2 HIS B   9    21.915  17.007 -14.589  1.00 28.09       B
ATOM   2921  ND1 HIS B   9    22.466  15.056 -13.780  1.00 26.71       B
ATOM   2922  CE1 HIS B   9    23.377  15.920 -13.367  1.00 27.14       B
ATOM   2923  NE2 HIS B   9    23.064  17.114 -13.843  1.00 29.19       B
ATOM   2924  C   HIS B   9    18.460  15.284 -13.250  1.00 22.99       B
ATOM   2925  O   HIS B   9    18.789  15.913 -12.229  1.00 23.60       B
ATOM   2926  N   LEU B  10    17.222  15.347 -13.737  1.00 21.72       B
ATOM   2927  CA  LEU B  10    16.202  16.182 -13.157  1.00 21.01       B
ATOM   2928  CB  LEU B  10    15.454  16.876 -14.310  1.00 21.10       B
ATOM   2929  CG  LEU B  10    14.381  17.868 -13.903  1.00 19.07       B
ATOM   2930  CD1 LEU B  10    15.051  19.052 -13.212  1.00 20.85       B
ATOM   2931  CD2 LEU B  10    13.613  18.369 -15.152  1.00 18.56       B
ATOM   2932  C   LEU B  10    15.181  15.513 -12.200  1.00 22.03       B
ATOM   2933  O   LEU B  10    14.732  16.119 -11.216  1.00 23.32       B
ATOM   2934  N   LEU B  11    14.860  14.247 -12.460  1.00 19.50       B
ATOM   2935  CA  LEU B  11    13.848  13.520 -11.718  1.00 21.06       B
ATOM   2936  CB  LEU B  11    13.667  12.159 -12.376  1.00 21.78       B
ATOM   2937  CG  LEU B  11    12.270  11.573 -12.315  1.00 23.01       B
ATOM   2938  CD1 LEU B  11    11.245  12.601 -12.812  1.00 26.14       B
ATOM   2939  CD2 LEU B  11    12.219  10.366 -13.214  1.00 26.14       B
ATOM   2940  C   LEU B  11    13.979  13.363 -10.192  1.00 21.79       B
ATOM   2941  O   LEU B  11    13.053  13.717  -9.453  1.00 21.56       B
ATOM   2942  N   LYS B  12    15.095  12.826  -9.717  1.00 23.82       B
ATOM   2943  CA  LYS B  12    15.250  12.672  -8.267  1.00 24.71       B
ATOM   2944  CB  LYS B  12    16.543  11.923  -7.915  1.00 28.61       B
ATOM   2945  CG  LYS B  12    16.608  11.564  -6.431  1.00 31.97       B
ATOM   2946  CD  LYS B  12    17.856  10.741  -6.085  1.00 36.79       B
ATOM   2947  CE  LYS B  12    17.795  10.213  -4.650  1.00 37.65       B
ATOM   2948  NZ  LYS B  12    17.449  11.262  -3.640  1.00 39.04       B
ATOM   2949  C   LYS B  12    15.224  14.040  -7.576  1.00 22.39       B
ATOM   2950  O   LYS B  12    14.586  14.193  -6.542  1.00 22.26       B
ATOM   2951  N   PRO B  13    15.932  15.052  -8.123  1.00 20.35       B
ATOM   2952  CD  PRO B  13    17.026  15.053  -9.103  1.00 19.55       B
ATOM   2953  CA  PRO B  13    15.855  16.346  -7.434  1.00 19.49       B
ATOM   2954  CB  PRO B  13    16.669  17.272  -8.333  1.00 19.36       B
ATOM   2955  CG  PRO B  13    17.750  16.376  -8.827  1.00 19.86       B
ATOM   2956  C   PRO B  13    14.420  16.838  -7.294  1.00 19.87       B
ATOM   2957  O   PRO B  13    14.041  17.346  -6.250  1.00 17.95       B
ATOM   2958  N   LEU B  14    13.620  16.710  -8.363  1.00 18.71       B
ATOM   2959  CA  LEU B  14    12.231  17.130  -8.294  1.00 22.23       B
ATOM   2960  CB  LEU B  14    11.532  16.907  -9.641  1.00 21.65       B
ATOM   2961  CG  LEU B  14    11.656  17.995 -10.680  1.00 20.62       B
ATOM   2962  CD1 LEU B  14    10.975  17.528 -11.993  1.00 18.11       B
ATOM   2963  CD2 LEU B  14    11.024  19.287 -10.152  1.00 20.79       B
ATOM   2964  C   LEU B  14    11.464  16.390  -7.215  1.00 22.60       B
ATOM   2965  O   LEU B  14    10.644  16.963  -6.504  1.00 23.92       B
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Figure 1 (continued 30)

ATOM	2966	N	GLN	B	15	11.720	15.091	-7.121	1.00	24.48	B
ATOM	2967	CA	GLN	B	15	11.053	14.254	-6.149	1.00	25.57	B
ATOM	2968	CB	GLN	B	15	11.481	12.808	-6.340	1.00	28.51	B
ATOM	2969	CG	GLN	B	15	10.827	11.860	-5.383	1.00	32.34	B
ATOM	2970	CD	GLN	B	15	11.261	10.436	-5.657	1.00	35.26	B
ATOM	2971	OE1	GLN	B	15	11.086	9.924	-6.769	1.00	36.87	B
ATOM	2972	NE2	GLN	B	15	11.841	9.789	-4.651	1.00	37.81	B
ATOM	2973	C	GLN	B	15	11.402	14.692	-4.746	1.00	25.12	B
ATOM	2974	O	GLN	B	15	10.546	14.800	-3.872	1.00	24.87	B
ATOM	2975	N	GLN	B	16	12.685	14.941	-4.533	1.00	23.65	B
ATOM	2976	CA	GLN	B	16	13.133	15.374	-3.224	1.00	23.01	B
ATOM	2977	CB	GLN	B	16	14.649	15.351	-3.161	1.00	26.68	B
ATOM	2978	CG	GLN	B	16	15.220	13.938	-3.057	1.00	33.06	B
ATOM	2979	CD	GLN	B	16	15.149	13.363	-1.639	1.00	34.57	B
ATOM	2980	OE1	GLN	B	16	15.499	12.208	-1.417	1.00	37.92	B
ATOM	2981	NE2	GLN	B	16	14.709	14.170	-0.683	1.00	36.18	B
ATOM	2982	C	GLN	B	16	12.640	16.761	-2.798	1.00	22.25	B
ATOM	2983	O	GLN	B	16	12.218	16.966	-1.657	1.00	21.67	B
ATOM	2984	N	VAL	B	17	12.665	17.731	-3.697	1.00	19.74	B
ATOM	2985	CA	VAL	B	17	12.234	19.045	-3.234	1.00	21.71	B
ATOM	2986	CB	VAL	B	17	12.701	20.165	-4.175	1.00	21.43	B
ATOM	2987	CG1	VAL	B	17	14.229	20.161	-4.234	1.00	21.95	B
ATOM	2988	CG2	VAL	B	17	12.098	20.000	-5.563	1.00	17.76	B
ATOM	2989	C	VAL	B	17	10.738	19.160	-3.002	1.00	21.93	B
ATOM	2990	O	VAL	B	17	10.278	20.075	-2.330	1.00	23.73	B
ATOM	2991	N	SER	B	18	9.993	18.221	-3.545	1.00	23.91	B
ATOM	2992	CA	SER	B	18	8.548	18.205	-3.374	1.00	25.13	B
ATOM	2993	CB	SER	B	18	7.923	17.397	-4.502	1.00	25.03	B
ATOM	2994	OG	SER	B	18	8.075	18.078	-5.727	1.00	24.69	B
ATOM	2995	C	SER	B	18	8.092	17.636	-2.024	1.00	26.98	B
ATOM	2996	O	SER	B	18	6.926	17.771	-1.660	1.00	27.31	B
ATOM	2997	N	GLY	B	19	9.017	17.010	-1.300	1.00	26.53	B
ATOM	2998	CA	GLY	B	19	8.706	16.413	-0.012	1.00	27.63	B
ATOM	2999	C	GLY	B	19	7.842	17.206	0.951	1.00	27.65	B
ATOM	3000	O	GLY	B	19	6.788	16.717	1.364	1.00	27.01	B
ATOM	3001	N	PRO	B	20	8.265	18.416	1.351	1.00	28.69	B
ATOM	3002	CD	PRO	B	20	9.611	18.974	1.119	1.00	30.14	B
ATOM	3003	CA	PRO	B	20	7.499	19.255	2.288	1.00	29.93	B
ATOM	3004	CB	PRO	B	20	8.462	20.415	2.594	1.00	30.20	B
ATOM	3005	CG	PRO	B	20	9.415	20.424	1.436	1.00	30.31	B
ATOM	3006	C	PRO	B	20	6.111	19.744	1.848	1.00	31.66	B
ATOM	3007	O	PRO	B	20	5.360	20.297	2.650	1.00	32.04	B
ATOM	3008	N	LEU	B	21	5.759	19.532	0.585	1.00	33.35	B
ATOM	3009	CA	LEU	B	21	4.456	19.982	0.089	1.00	34.98	B
ATOM	3010	CB	LEU	B	21	4.506	20.208	-1.429	1.00	33.56	B
ATOM	3011	CG	LEU	B	21	5.187	21.476	-1.954	1.00	33.69	B
ATOM	3012	CD1	LEU	B	21	6.657	21.499	-1.573	1.00	32.31	B
ATOM	3013	CD2	LEU	B	21	5.034	21.520	-3.473	1.00	33.19	B
ATOM	3014	C	LEU	B	21	3.331	19.003	0.412	1.00	36.25	B
ATOM	3015	O	LEU	B	21	3.543	17.799	0.452	1.00	37.14	B
ATOM	3016	N	GLY	B	22	2.132	19.540	0.636	1.00	38.77	B
ATOM	3017	CA	GLY	B	22	0.982	18.707	0.941	1.00	40.45	B
ATOM	3018	C	GLY	B	22	0.122	18.423	-0.278	1.00	41.62	B
ATOM	3019	O	GLY	B	22	0.323	19.015	-1.348	1.00	42.14	B
ATOM	3020	N	GLY	B	23	-0.840	17.516	-0.117	1.00	42.36	B
ATOM	3021	CA	GLY	B	23	-1.731	17.170	-1.214	1.00	42.80	B
ATOM	3022	C	GLY	B	23	-2.597	18.349	-1.621	1.00	42.52	B
ATOM	3023	O	GLY	B	23	-3.006	18.470	-2.776	1.00	42.78	B
ATOM	3024	N	ARG	B	24	-2.886	19.223	-0.664	1.00	42.28	B
ATOM	3025	CA	ARG	B	24	-3.691	20.400	-0.951	1.00	41.15	B
ATOM	3026	CB	ARG	B	24	-5.114	20.240	-0.419	1.00	44.69	B
ATOM	3027	CG	ARG	B	24	-6.032	21.311	-0.973	1.00	48.56	B
ATOM	3028	CD	ARG	B	24	-7.337	21.431	-0.212	1.00	52.31	B
ATOM	3029	NE	ARG	B	24	-8.207	22.431	-0.831	1.00	55.67	B
ATOM	3030	CZ	ARG	B	24	-7.851	23.690	-1.079	1.00	57.36	B
ATOM	3031	NH1	ARG	B	24	-6.634	24.122	-0.760	1.00	58.66	B
ATOM	3032	NH2	ARG	B	24	-8.711	24.521	-1.656	1.00	58.21	B
ATOM	3033	C	ARG	B	24	-3.067	21.645	-0.332	1.00	38.07	B
ATOM	3034	O	ARG	B	24	-3.273	21.934	0.845	1.00	38.01	B
ATOM	3035	N	PRO	B	25	-2.295	22.401	-1.124	1.00	35.11	B
ATOM	3036	CD	PRO	B	25	-2.021	22.244	-2.565	1.00	34.80	B
ATOM	3037	CA	PRO	B	25	-1.663	23.611	-0.601	1.00	32.06	B
ATOM	3038	CB	PRO	B	25	-0.820	24.099	-1.779	1.00	31.38	B
ATOM	3039	CG	PRO	B	25	-1.619	23.646	-2.967	1.00	33.86	B
ATOM	3040	C	PRO	B	25	-2.692	24.634	-0.147	1.00	29.51	B
ATOM	3041	O	PRO	B	25	-3.711	24.864	-0.803	1.00	28.23	B
ATOM	3042	N	THR	B	26	-2.412	25.236	0.996	1.00	28.41	B
ATOM	3043	CA	THR	B	26	-3.285	26.240	1.565	1.00	27.34	B
ATOM	3044	CB	THR	B	26	-2.673	26.762	2.861	1.00	28.45	B
ATOM	3045	OG1	THR	B	26	-2.397	25.643	3.717	1.00	31.15	B
ATOM	3046	CG2	THR	B	26	-3.626	27.732	3.546	1.00	28.57	B
ATOM	3047	C	THR	B	26	-3.504	27.389	0.587	1.00	25.70	B
ATOM	3048	O	THR	B	26	-4.624	27.893	0.428	1.00	27.11	B
ATOM	3049	N	LEU	B	27	-2.426	27.829	-0.044	1.00	23.09	B
ATOM	3050	CA	LEU	B	27	-2.507	28.881	-1.043	1.00	21.25	B
ATOM	3051	CB	LEU	B	27	-1.953	30.195	-0.511	1.00	21.63	B
ATOM	3052	CG	LEU	B	27	-2.900	30.896	0.483	1.00	23.04	B
ATOM	3053	CD1	LEU	B	27	-2.264	32.203	0.895	1.00	24.85	B
ATOM	3054	CD2	LEU	B	27	-4.270	31.144	-0.160	1.00	24.74	B
ATOM	3055	C	LEU	B	27	-1.718	28.392	-2.247	1.00	20.78	B
ATOM	3056	O	LEU	B	27	-0.775	27.601	-2.105	1.00	17.68	B
ATOM	3057	N	PRO	B	28	-2.084	28.863	-3.443	1.00	18.82	B
ATOM	3058	CD	PRO	B	28	-3.104	29.903	-3.700	1.00	18.71	B
ATOM	3059	CA	PRO	B	28	-1.413	28.443	-4.682	1.00	18.57	B
ATOM	3060	CB	PRO	B	28	-1.917	29.446	-5.722	1.00	20.77	B
ATOM	3061	CG	PRO	B	28	-3.292	29.834	-5.195	1.00	20.10	B
ATOM	3062	C	PRO	B	28	0.110	28.355	-4.684	1.00	18.35	B
ATOM	3063	O	PRO	B	28	0.666	27.322	-5.114	1.00	16.61	B
ATOM	3064	N	ILE	B	29	0.781	29.409	-4.230	1.00	16.22	B
ATOM	3065	CA	ILE	B	29	2.257	29.431	-4.241	1.00	17.45	B

Figure 1 (continued 31)

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ATOM   3066  CB   ILE B  29      2.810  30.770  -3.637  1.00  19.27      B
ATOM   3067  CG2  ILE B  29      2.555  30.812  -2.154  1.00  20.68      B
ATOM   3068  CG1  ILE B  29      4.304  30.917  -3.901  1.00  23.27      B
ATOM   3069  CD1  ILE B  29      4.653  31.204  -5.338  1.00  22.71      B
ATOM   3070  C    ILE B  29      2.880  28.264  -3.502  1.00  15.97      B
ATOM   3071  O    ILE B  29      3.957  27.778  -3.907  1.00  14.64      B
ATOM   3072  N    LEU B  30      2.218  27.775  -2.452  1.00  16.95      B
ATOM   3073  CA   LEU B  30      2.782  26.670  -1.664  1.00  16.78      B
ATOM   3074  CB   LEU B  30      2.094  26.575  -0.300  1.00  18.79      B
ATOM   3075  CG   LEU B  30      2.283  27.856   0.524  1.00  19.43      B
ATOM   3076  CD1  LEU B  30      1.556.  27.675   1.859  1.00  19.92      B
ATOM   3077  CD2  LEU B  30      3.728  28.159   0.783  1.00  18.87      B
ATOM   3078  C    LEU B  30      2.752  25.322  -2.374  1.00  17.78      B
ATOM   3079  O    LEU B  30      3.343  24.340  -1.901  1.00  18.71      B
ATOM   3080  N    GLY B  31      2.066  25.280  -3.505  1.00  14.09      B
ATOM   3081  CA   GLY B  31      1.999  24.068  -4.318  1.00  15.57      B
ATOM   3082  C    GLY B  31      2.992  24.160  -5.466  1.00  13.53      B
ATOM   3083  O    GLY B  31      3.038  23.269  -6.317  1.00  15.55      B
ATOM   3084  N    ASN B  32      3.796  25.200  -5.476  1.00  12.64      B
ATOM   3085  CA   ASN B  32      4.767  25.400  -6.551  1.00  12.56      B
ATOM   3086  CB   ASN B  32      4.690  26.838  -7.107  1.00  12.94      B
ATOM   3087  CG   ASN B  32      3.502  27.045  -8.024  1.00  10.96      B
ATOM   3088  OD1  ASN B  32      2.599  26.224  -8.085  1.00  12.20      B
ATOM   3089  ND2  ASN B  32      3.523  28.158  -8.771  1.00  13.16      B
ATOM   3090  C    ASN B  32      6.178  25.176  -6.075  1.00  14.19      B
ATOM   3091  O    ASN B  32      6.481  25.195  -4.868  1.00  14.24      B
ATOM   3092  N    LEU B  33      7.050  24.957  -7.052  1.00  13.85      B
ATOM   3093  CA   LEU B  33      8.459  24.861  -6.774  1.00  13.97      B
ATOM   3094  CB   LEU B  33      9.097  23.641  -7.433  1.00  15.40      B
ATOM   3095  CG   LEU B  33      8.586  22.254  -7.072  1.00  17.90      B
ATOM   3096  CD1  LEU B  33      9.410  21.226  -7.867  1.00  18.49      B
ATOM   3097  CD2  LEU B  33      8.782  22.024  -5.568  1.00  19.70      B
ATOM   3098  C    LEU B  33      9.115  26.086  -7.395  1.00  13.05      B
ATOM   3099  O    LEU B  33      8.725  26.540  -8.465  1.00  13.07      B
ATOM   3100  N    LEU B  34     10.126  26.610  -6.722  1.00  12.75      B
ATOM   3101  CA   LEU B  34     10.895  27.732  -7.225  1.00  12.14      B
ATOM   3102  CB   LEU B  34     11.510  28.520  -6.056  1.00  13.47      B
ATOM   3103  CG   LEU B  34     12.562  29.560  -6.427  1.00  12.92      B
ATOM   3104  CD1  LEU B  34     11.973  30.697  -7.293  1.00  14.04      B
ATOM   3105  CD2  LEU B  34     13.130  30.156  -5.123  1.00  14.82      B
ATOM   3106  C    LEU B  34     12.029  27.176  -8.099  1.00  13.14      B
ATOM   3107  O    LEU B  34     12.760  26.275  -7.652  1.00  12.90      B
ATOM   3108  N    LEU B  35     12.125  27.651  -9.351  1.00  11.64      B
ATOM   3109  CA   LEU B  35     13.187  27.245 -10.291  1.00  11.91      B
ATOM   3110  CB   LEU B  35     12.615  26.811 -11.669  1.00  11.42      B
ATOM   3111  CG   LEU B  35     12.046  25.413 -11.738  1.00  14.74      B
ATOM   3112  CD1  LEU B  35     11.127  25.120 -10.596  1.00  18.38      B
ATOM   3113  CD2  LEU B  35     11.288  25.299 -13.074  1.00  15.91      B
ATOM   3114  C    LEU B  35     14.071  28.445 -10.542  1.00  13.47      B
ATOM   3115  O    LEU B  35     13.573  29.535 -10.900  1.00  14.51      B
ATOM   3116  N    GLN B  36     15.376  28.285 -10.350  1.00  13.11      B
ATOM   3117  CA   GLN B  36     16.300  29.400 -10.578  1.00  13.83      B
ATOM   3118  CB   GLN B  36     16.806  29.935  -9.223  1.00  16.19      B
ATOM   3119  CG   GLN B  36     15.726  30.383  -8.281  1.00  16.86      B
ATOM   3120  CD   GLN B  36     16.264  30.626  -6.866  1.00  21.22      B
ATOM   3121  OE1  GLN B  36     16.232  31.760  -6.363  1.00  25.16      B
ATOM   3122  NE2  GLN B  36     16.770  29.570  -6.229  1.00  16.45      B
ATOM   3123  C    GLN B  36     17.495  28.935 -11.376  1.00  13.60      B
ATOM   3124  O    GLN B  36     18.135  27.952 -10.993  1.00  14.49      B
ATOM   3125  N    VAL B  37     17.810  29.640 -12.474  1.00  11.56      B
ATOM   3126  CA   VAL B  37     18.997  29.285 -13.248  1.00  13.61      B
ATOM   3127  CB   VAL B  37     18.731  29.191 -14.777  1.00  12.84      B
ATOM   3128  CG1  VAL B  37     20.074  29.020 -15.553  1.00  14.43      B
ATOM   3129  CG2  VAL B  37     17.804  27.985 -15.051  1.00  14.23      B
ATOM   3130  C    VAL B  37     19.965  30.435 -13.005  1.00  15.18      B
ATOM   3131  O    VAL B  37     19.611  31.603 -13.228  1.00  15.34      B
ATOM   3132  N    ALA B  38     21.139  30.117 -12.472  1.00  15.02      B
ATOM   3133  CA   ALA B  38     22.161  31.146 -12.227  1.00  15.51      B
ATOM   3134  CB   ALA B  38     21.954  31.783 -10.878  1.00  15.09      B
ATOM   3135  C    ALA B  38     23.493  30.446 -12.291  1.00  19.33      B
ATOM   3136  O    ALA B  38     23.644  29.366 -11.747  1.00  18.26      B
ATOM   3137  N    ASP B  39     24.473  31.060 -12.953  1.00  22.66      B
ATOM   3138  CA   ASP B  39     25.765  30.393 -13.153  1.00  26.58      B
ATOM   3139  CB   ASP B  39     26.389  29.982 -11.829  1.00  32.37      B
ATOM   3140  CG   ASP B  39     27.184  31.097 -11.201  1.00  36.57      B
ATOM   3141  OD1  ASP B  39     28.336  31.328 -11.655  1.00  39.34      B
ATOM   3142  OD2  ASP B  39     26.658  31.756 -10.270  1.00  38.78      B
ATOM   3143  C    ASP B  39     25.429  29.150 -13.986  1.00  26.82      B
ATOM   3144  O    ASP B  39     24.550  29.189 -14.844  1.00  29.26      B
ATOM   3145  N    GLY B  40     26.080  28.031 -13.733  1.00  26.59      B
ATOM   3146  CA   GLY B  40     25.759  26.871 -14.539  1.00  23.64      B
ATOM   3147  C    GLY B  40     24.910  25.927 -13.730  1.00  19.76      B
ATOM   3148  O    GLY B  40     25.044  24.723 -13.871  1.00  20.20      B
ATOM   3149  N    THR B  41     24.046  26.498 -12.883  1.00  18.09      B
ATOM   3150  CA   THR B  41     23.215  25.701 -11.983  1.00  15.70      B
ATOM   3151  CB   THR B  41     23.684  25.916 -10.551  1.00  16.47      B
ATOM   3152  OG1  THR B  41     25.090  25.633 -10.486  1.00  19.61      B
ATOM   3153  CG2  THR B  41     22.918  25.016  -9.549  1.00  17.43      B
ATOM   3154  C    THR B  41     21.721  25.988 -11.974  1.00  13.03      B
ATOM   3155  O    THR B  41     21.308  27.129 -11.944  1.00  14.12      B
ATOM   3156  N    LEU B  42     20.924  24.933 -12.005  1.00  13.26      B
ATOM   3157  CA   LEU B  42     19.483  25.093 -11.850  1.00  11.94      B
ATOM   3158  CB   LEU B  42     18.743  24.061 -12.723  1.00  11.39      B
ATOM   3159  CG   LEU B  42     17.292  23.803 -12.339  1.00  10.89      B
ATOM   3160  CD1  LEU B  42     16.422  25.083 -12.504  1.00  13.06      B
ATOM   3161  CD2  LEU B  42     16.760  22.694 -13.241  1.00  12.39      B
ATOM   3162  C    LEU B  42     19.222  24.731 -10.385  1.00  12.70      B
ATOM   3163  O    LEU B  42     19.633  23.642  -9.935  1.00  13.40      B
ATOM   3164  N    SER B  43     18.551  25.613  -9.641  1.00  10.83      B
ATOM   3165  CA   SER B  43     18.212  25.317  -8.240  1.00  13.03      B
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Figure 1 (continued 32)

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ATOM   3166  CB   SER B  43     18.605  26.457  -7.298  1.00 15.48      B
ATOM   3167  OG   SER B  43     20.017  26.635  -7.258  1.00 16.36      B
ATOM   3168  C    SER B  43     16.699  25.141  -8.194  1.00 12.37      B
ATOM   3169  O    SER B  43     15.953  25.873  -8.875  1.00 13.81      B
ATOM   3170  N    LEU B  44     16.259  24.133  -7.427  1.00 12.48      B
ATOM   3171  CA   LEU B  44     14.832  23.840  -7.249  1.00 11.34      B
ATOM   3172  CB   LEU B  44     14.504  22.413  -7.724  1.00 12.56      B
ATOM   3173  CG   LEU B  44     14.993  22.028  -9.122  1.00 14.70      B
ATOM   3174  CD1  LEU B  44     14.964  20.500  -9.306  1.00 18.40      B
ATOM   3175  CD2  LEU B  44     14.105  22.717 -10.133  1.00 19.25      B
ATOM   3176  C    LEU B  44     14.581  23.918  -5.746  1.00 13.84      B
ATOM   3177  O    LEU B  44     15.344  23.356  -4.936  1.00 12.96      B
ATOM   3178  N    THR B  45     13.499  24.583  -5.359  1.00 11.87      B
ATOM   3179  CA   THR B  45     13.179  24.726  -3.928  1.00 13.31      B
ATOM   3180  CB   THR B  45     13.481  26.166  -3.421  1.00 13.75      B
ATOM   3181  OG1  THR B  45     14.869  26.485  -3.627  1.00 15.13      B
ATOM   3182  CG2  THR B  45     13.157  26.269  -1.922  1.00 14.06      B
ATOM   3183  C    THR B  45     11.698  24.477  -3.666  1.00 14.00      B
ATOM   3184  O    THR B  45     10.867  24.948  -4.423  1.00 13.55      B
ATOM   3185  N    GLY B  46     11.396  23.696  -2.631  1.00 13.36      B
ATOM   3186  CA   GLY B  46     10.029  23.408  -2.203  1.00 13.22      B
ATOM   3187  C    GLY B  46      9.898  23.843  -0.738  1.00 14.39      B
ATOM   3188  O    GLY B  46     10.856  23.711   0.017  1.00 15.56      B
ATOM   3189  N    THR B  47      8.736  24.387  -0.333  1.00 14.57      B
ATOM   3190  CA   THR B  47      8.592  24.822   1.061  1.00 15.34      B
ATOM   3191  CB   THR B  47      8.985  26.317   1.236  1.00 16.19      B
ATOM   3192  OG1  THR B  47      9.049  26.655   2.632  1.00 15.79      B
ATOM   3193  CG2  THR B  47      7.967  27.253   0.564  1.00 17.31      B
ATOM   3194  C    THR B  47      7.162  24.668   1.564  1.00 16.59      B
ATOM   3195  O    THR B  47      6.226  24.562   0.768  1.00 16.42      B
ATOM   3196  N    ASP B  48      7.009  24.615   2.887  1.00 17.13      B
ATOM   3197  CA   ASP B  48      5.658  24.598   3.487  1.00 16.11      B
ATOM   3198  CB   ASP B  48      5.344  23.244   4.132  1.00 15.80      B
ATOM   3199  CG   ASP B  48      6.136  22.986   5.398  1.00 16.28      B
ATOM   3200  OD1  ASP B  48      7.041  23.773   5.722  1.00 16.79      B
ATOM   3201  OD2  ASP B  48      5.825  21.976   6.074  1.00 20.58      B
ATOM   3202  C    ASP B  48      5.559  25.736   4.521  1.00 18.07      B
ATOM   3203  O    ASP B  48      4.612  25.768   5.321  1.00 18.39      B
ATOM   3204  N    LEU B  49      6.545  26.641   4.479  1.00 15.86      B
ATOM   3205  CA   LEU B  49      6.712  27.827   5.343  1.00 17.77      B
ATOM   3206  CB   LEU B  49      5.383  28.520   5.666  1.00 17.51      B
ATOM   3207  CG   LEU B  49      4.676  29.110   4.453  1.00 17.64      B
ATOM   3208  CD1  LEU B  49      3.373  29.816   4.956  1.00 21.50      B
ATOM   3209  CD2  LEU B  49      5.594  30.102   3.756  1.00 19.20      B
ATOM   3210  C    LEU B  49      7.406  27.475   6.656  1.00 16.84      B
ATOM   3211  O    LEU B  49      7.860  28.372   7.370  1.00 20.06      B
ATOM   3212  N    GLU B  50      7.467  26.189   6.991  1.00 17.57      B
ATOM   3213  CA   GLU B  50      8.164  25.802   8.228  1.00 16.55      B
ATOM   3214  CB   GLU B  50      7.359  24.747   9.000  1.00 20.80      B
ATOM   3215  CG   GLU B  50      7.969  24.377  10.373  1.00 25.34      B
ATOM   3216  CD   GLU B  50      7.109  23.396  11.186  1.00 29.02      B
ATOM   3217  OE1  GLU B  50      7.079  23.504  12.435  1.00 30.09      B
ATOM   3218  OE2  GLU B  50      6.487  22.496  10.592  1.00 31.29      B
ATOM   3219  C    GLU B  50      9.540  25.238   7.842  1.00 16.32      B
ATOM   3220  O    GLU B  50     10.511  25.373   8.580  1.00 16.99      B
ATOM   3221  N    MET B  51      9.611  24.630   6.672  1.00 15.47      B
ATOM   3222  CA   MET B  51     10.882  24.074   6.215  1.00 14.90      B
ATOM   3223  CB   MET B  51     10.987  22.609   6.653  1.00 15.67      B
ATOM   3224  CG   MET B  51      9.910  21.720   6.114  1.00 17.25      B
ATOM   3225  SD   MET B  51      9.719  20.228   7.113  1.00 21.05      B
ATOM   3226  CE   MET B  51      8.965  20.945   8.604  1.00 23.10      B
ATOM   3227  C    MET B  51     10.988  24.187   4.721  1.00 14.86      B
ATOM   3228  O    MET B  51      9.978  24.437   4.029  1.00 15.26      B
ATOM   3229  N    GLU B  52     12.210  24.027   4.202  1.00 14.83      B
ATOM   3230  CA   GLU B  52     12.367  24.087   2.755  1.00 13.34      B
ATOM   3231  CB   GLU B  52     12.761  25.477   2.295  1.00 18.93      B
ATOM   3232  CG   GLU B  52     13.998  26.005   2.925  1.00 25.39      B
ATOM   3233  CD   GLU B  52     14.361  27.374   2.411  1.00 31.84      B
ATOM   3234  OE1  GLU B  52     13.504  28.295   2.473  1.00 32.96     \B
ATOM   3235  OE2  GLU B  52     15.520  27.508   1.960  1.00 35.26     !B
ATOM   3236  C    GLU B  52     13.420  23.100   2.339  1.00 14.63      B
ATOM   3237  O    GLU B  52     14.317  22.798   3.108  1.00 14.47      B
ATOM   3238  N    MET B  53     13.314  22.604   1.117  1.00 13.33      B
ATOM   3239  CA   MET B  53     14.280  21.636   0.610  1.00 14.02      B
ATOM   3240  CB   MET B  53     13.575  20.289   0.379  1.00 16.35      B
ATOM   3241  CG   MET B  53     14.496  19.209  -0.220  1.00 19.16      B
ATOM   3242  SD   MET B  53     15.833  18.696   0.914  1.00 23.65      B
ATOM   3243  CE   MET B  53     14.878  17.649   1.951  1.00 20.87      B
ATOM   3244  C    MET B  53     14.777  22.225  -0.701  1.00 14.06      B
ATOM   3245  O    MET B  53     13.977  22.607  -1.546  1.00 13.90      B
ATOM   3246  N    VAL B  54     16.091  22.294  -0.872  1.00 13.10      B
ATOM   3247  CA   VAL B  54     16.687  22.882  -2.089  1.00 13.22      B
ATOM   3248  CB   VAL B  54     17.539  24.079  -1.725  1.00 14.45      B
ATOM   3249  CG1  VAL B  54     18.117  24.704  -2.984  1.00 14.52      B
ATOM   3250  CG2  VAL B  54     16.699  25.088  -0.938  1.00 13.15      B
ATOM   3251  C    VAL B  54     17.590  21.867  -2.768  1.00 13.82      B
ATOM   3252  O    VAL B  54     18.330  21.169  -2.093  1.00 16.01      B
ATOM   3253  N    ALA B  55     17.513  21.765  -4.096  1.00 11.25      B
ATOM   3254  CA   ALA B  55     18.380  20.865  -4.850  1.00 13.21      B
ATOM   3255  CB   ALA B  55     17.548  19.820  -5.605  1.00 12.81      B
ATOM   3256  C    ALA B  55     19.144  21.706  -5.863  1.00 15.53      B
ATOM   3257  O    ALA B  55     18.564  22.606  -6.461  1.00 15.73      B
ATOM   3258  N    ARG B  56     20.433  21.410  -6.059  1.00 14.23      B
ATOM   3259  CA   ARG B  56     21.258  22.119  -7.044  1.00 15.31      B
ATOM   3260  CB   ARG B  56     22.601  22.523  -6.432  1.00 16.38      B
ATOM   3261  CG   ARG B  56     22.482  23.229  -5.112  1.00 22.20      B
ATOM   3262  CD   ARG B  56     22.101  24.643  -5.283  1.00 24.40      B
ATOM   3263  NE   ARG B  56     22.131  25.327  -3.990  1.00 26.52      B
ATOM   3264  CZ   ARG B  56     21.494  26.463  -3.729  1.00 27.62      B
ATOM   3265  NH1  ARG B  56     20.779  27.069  -4.676  1.00 23.46      B
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Figure 1 (continued 33)

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ATOM   3266   NH2  ARG B   56      21.523  26.966   -2.496  1.00  28.24        B
ATOM   3267   C    ARG B   56      21.525  21.120   -8.158  1.00  14.84        B
ATOM   3268   O    ARG B   56      21.995  19.996   -7.905  1.00  16.83        B
ATOM   3269   N    VAL B   57      21.203  21.504   -9.387  1.00  13.57        B
ATOM   3270   CA   VAL B   57      21.402  20.616  -10.511  1.00  15.14        B
ATOM   3271   CB   VAL B   57      20.049  20.326  -11.197  1.00  17.22        B
ATOM   3272   CG1  VAL B   57      20.238  19.426  -12.403  1.00  17.28        B
ATOM   3273   CG2  VAL B   57      19.076  19.642  -10.185  1.00  16.94        B
ATOM   3274   C    VAL B   57      22.378  21.261  -11.510  1.00  14.02        B
ATOM   3275   O    VAL B   57      22.090  22.326  -12.063  1.00  15.02        B
ATOM   3276   N    ALA B   58      23.495  20.589  -11.786  1.00  15.91        B
ATOM   3277   CA   ALA B   58      24.457  21.141  -12.749  1.00  15.97        B
ATOM   3278   CB   ALA B   58      25.763  20.328  -12.705  1.00  16.60        B
ATOM   3279   C    ALA B   58      23.883  21.096  -14.178  1.00  15.88        B
ATOM   3280   O    ALA B   58      23.266  20.118  -14.569  1.00  16.91        B
ATOM   3281   N    LEU B   59      24.106  22.157  -14.947  1.00  13.80        B
ATOM   3282   CA   LEU B   59      23.618  22.249  -16.321  1.00  13.84        B
ATOM   3283   CB   LEU B   59      22.888  23.587  -16.527  1.00  14.79        B
ATOM   3284   CG   LEU B   59      21.708  23.860  -15.578  1.00  13.18        B
ATOM   3285   CD1  LEU B   59      21.112  25.257  -15.826  1.00  16.02        B
ATOM   3286   CD2  LEU B   59      20.641  22.815  -15.803  1.00  13.77        B
ATOM   3287   C    LEU B   59      24.820  22.178  -17.264  1.00  16.59        B
ATOM   3288   O    LEU B   59      25.670  23.089  -17.254  1.00  18.41        B
ATOM   3289   N    VAL B   60      24.906  21.037  -18.037  1.00  16.00        B
ATOM   3290   CA   VAL B   60      25.987  20.866  -19.030  1.00  16.12        B
ATOM   3291   CB   VAL B   60      26.497  19.402  -19.011  1.00  17.87        B
ATOM   3292   CG1  VAL B   60      27.080  19.074  -17.627  1.00  17.15        B
ATOM   3293   CG2  VAL B   60      25.361  18.434  -19.397  1.00  15.97        B
ATOM   3294   C    VAL B   60      25.541  21.219  -20.443  1.00  18.35        B
ATOM   3295   O    VAL B   60      26.366  21.214  -21.382  1.00  18.50        B
ATOM   3296   N    GLN B   61      24.259  21.561  -20.617  1.00  17.91        B
ATOM   3297   CA   GLN B   61      23.731  21.970  -21.926  1.00  18.15        B
ATOM   3298   CB   GLN B   61      22.400  21.256  -22.242  1.00  17.50        B
ATOM   3299   CG   GLN B   61      22.541  19.751  -22.248  1.00  17.69        B
ATOM   3300   CD   GLN B   61      21.298  19.043  -22.798  1.00  14.84        B
ATOM   3301   OE1  GLN B   61      20.828  19.336  -23.922  1.00  16.87        B
ATOM   3302   NE2  GLN B   61      20.776  18.097  -22.026  1.00  16.99        B
ATOM   3303   C    GLN B   61      23.478  23.468  -21.873  1.00  19.28        B
ATOM   3304   O    GLN B   61      23.366  24.020  -20.778  1.00  17.31        B
ATOM   3305   N    PRO B   62      23.351  24.125  -23.046  1.00  18.68        B
ATOM   3306   CD   PRO B   62      23.472  23.548  -24.401  1.00  20.65        B
ATOM   3307   CA   PRO B   62      23.098  25.577  -23.114  1.00  19.82        B
ATOM   3308   CB   PRO B   62      22.828  25.809  -24.591  1.00  22.37        B
ATOM   3309   CG   PRO B   62      23.740  24.781  -25.242  1.00  21.05        B
ATOM   3310   C    PRO B   62      21.934  26.045  -22.220  1.00  19.61        B
ATOM   3311   O    PRO B   62      20.901  25.388  -22.159  1.00  19.83        B
ATOM   3312   N    HIS B   63      22.121  27.174  -21.533  1.00  16.71        B
ATOM   3313   CA   HIS B   63      21.102  27.720  -20.624  1.00  15.04        B
ATOM   3314   CB   HIS B   63      21.307  27.117  -19.223  1.00  16.87        B
ATOM   3315   CG   HIS B   63      22.718  27.225  -18.743  1.00  16.35        B
ATOM   3316   CD2  HIS B   63      23.352  28.194  -18.045  1.00  19.97        B
ATOM   3317   ND1  HIS B   63      23.674  26.284  -19.052  1.00  19.14        B
ATOM   3318   CE1  HIS B   63      24.844  26.671  -18.566  1.00  18.64        B
ATOM   3319   NE2  HIS B   63      24.676  27.828  -17.954  1.00  21.06        B
ATOM   3320   C    HIS B   63      21.120  29.242  -20.524  1.00  16.64        B
ATOM   3321   O    HIS B   63      22.102  29.903  -20.917  1.00  18.95        B
ATOM   3322   N    GLU B   64      20.043  29.811  -19.988  1.00  14.93        B
ATOM   3323   CA   GLU B   64      19.904  31.269  -19.792  1.00  16.90        B
ATOM   3324   CB   GLU B.  64      18.948  31.878  -20.827  1.00  20.34        B
ATOM   3325   CG   GLU B   64      19.523  31.891  -22.209  1.00  23.46        B
ATOM   3326   CD   GLU B   64      18.491  32.235  -23.268  1.00  28.27        B
ATOM   3327   OE1  GLU B   64      17.465  32.858  -22.936  1.00  28.18        B
ATOM   3328   OE2  GLU B   64      18.725  31.878  -24.441  1.00  30.88        B
ATOM   3329   C    GLU B   64      19.369  31.526  -18.386  1.00  16.81        B
ATOM   3330   O    GLU B   64      18.451  30.834  -17.941  1.00  16.15        B
ATOM   3331   N    PRO B   65      19.945  32.500  -17.653  1.00  15.86        B
ATOM   3332   CD   PRO B   65      21.078  33.356  -18.046  1.00  17.72        B
ATOM   3333   CA   PRO B   65      19.502  32.808  -16.292  1.00  15.04        B
ATOM   3334   CB   PRO B   65      20.587  33.780  -15.774  1.00  17.31        \B
ATOM   3335   CG   PRO B   65      21.018  34.457  -16.991  1.00  18.09        'B
ATOM   3336   C    PRO B   65      18.088  33.355  -16.113  1.00  15.66        B
ATOM   3337   O    PRO B   65      17.508  33.964  -17.024  1.00  16.81        B
ATOM   3338   N    GLY B   66      17.530  33.112  -14.930  1.00  14.69        B
ATOM   3339   CA   GLY B   66      16.200  33.578  -14.601  1.00  14.85        B
ATOM   3340   C    GLY B   66      15.477  32.710  -13.600  1.00  15.33        B
ATOM   3341   O    GLY B   66      16.001  31.653  -13.195  1.00  14.73        B
ATOM   3342   N    ALA B   67      14.286  33.140  -13.187  1.00  13.47        B
ATOM   3343   CA   ALA B   67      13.542  32.384  -12.182  1.00  14.65        B
ATOM   3344   CB   ALA B   67      13.917  32.882  -10.767  1.00  14.42        B
ATOM   3345   C    ALA B   67      12.054  32.455  -12.334  1.00  14.70        B
ATOM   3346   O    ALA B   67      11.505  33.439  -12.854  1.00  15.40        B
ATOM   3347   N    THR B   68      11.386  31.417  -11.857  1.00  13.62        B
ATOM   3348   CA   THR B   68       9.929  31.390  -11.878  1.00  13.91        B
ATOM   3349   CB   THR B   68       9.391  31.110  -13.317  1.00  14.48        B
ATOM   3350   OG1  THR B   68       7.963  31.295  -13.339  1.00  15.83        B
ATOM   3351   CG2  THR B   68       9.694  29.668  -13.731  1.00  16.00        B
ATOM   3352   C    THR B   68       9.472  30.302  -10.924  1.00  14.71        B
ATOM   3353   O    THR B   68      10.311  29.641  -10.323  1.00  15.32        B
ATOM   3354   N    THR B   69       8.167  30.162  -10.724  1.00  13.55        B
ATOM   3355   CA   THR B   69       7.636  29.056   -9.894  1.00  12.29        B
ATOM   3356   CB   THR B   69       7.048  29.522   -8.520  1.00  14.79        B
ATOM   3357   OG1  THR B   69       5.754  30.105   -8.695  1.00  15.03        B
ATOM   3358   CG2  THR B   69       7.983  30.537   -7.876  1.00  14.41        B
ATOM   3359   C    THR B   69       6.555  28.385  -10.714  1.00  14.44        B
ATOM   3360   O    THR B   69       5.847  29.055  -11.465  1.00  14.38        B
ATOM   3361   N    VAL B   70       6.458  27.063  -10.629  1.00  13.03        B
ATOM   3362   CA   VAL B   70       5.464  26.297  -11.370  1.00  12.62        B
ATOM   3363   CB   VAL B   70       6.044  25.655  -12.631  1.00  14.60        B
ATOM   3364   CG1  VAL B   70       6.340  26.733  -13.667  1.00  17.68        B
ATOM   3365   CG2  VAL B   70       7.284  24.840  -12.267  1.00  16.64        B
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<p style="text-align:center">Figure 1 (continued 34)</p>

ATOM	3366	C	VAL	B	70	4.913	25.183	-10.490	1.00	12.72	B
ATOM	3367	O	VAL	B	70	5.550	24.803	-9.489	1.00	12.07	B
ATOM	3368	N	PRO	B	71	3.734	24.651	-10.825	1.00	12.89	B
ATOM	3369	CD	PRO	B	71	2.872	25.050	-11.964	1.00	14.31	B
ATOM	3370	CA	PRO	B	71	3.129	23.572	-10.016	1.00	12.87	B
ATOM	3371	CB	PRO	B	71	1.845	23.239	-10.756	1.00	14.80	B
ATOM	3372	CG	PRO	B	71	1.522	24.614	-11.481	1.00	19.52	B
ATOM	3373	C	PRO	B	71	4.044	22.363	-9.848	1.00	12.82	B
ATOM	3374	O	PRO	B	71	4.480	21.743	-10.813	1.00	13.40	B
ATOM	3375	N	ALA	B	72	4.340	22.035	-8.599	1.00	11.96	B
ATOM	3376	CA	ALA	B	72	5.293	20.944	-8.344	1.00	11.56	B
ATOM	3377	CB	ALA	B	72	5.611	20.907	-6.847	1.00	12.77	B
ATOM	3378	C	ALA	B	72	4.857	19.587	-8.805	1.00	13.14	B
ATOM	3379	O	ALA	B	72	5.618	18.899	-9.515	1.00	11.71	B
ATOM	3380	N	ARG	B	73	3.654	19.178	-8.426	1.00	12.89	B
ATOM	3381	CA	ARG	B	73	3.155	17.856	-8.777	1.00	15.37	B
ATOM	3382	CB	ARG	B	73	1.769	17.634	-8.137	1.00	19.29	B
ATOM	3383	CG	ARG	B	73	1.189	16.241	-8.362	1.00	28.52	B
ATOM	3384	CD	ARG	B	73	2.091	15.198	-7.713	1.00	33.56	B
ATOM	3385	NE	ARG	B	73	1.915	13.882	-8.310	1.00	39.25	B
ATOM	3386	CZ	ARG	B	73	2.786	12.882	-8.182	1.00	39.95	B
ATOM	3387	NH1	ARG	B	73	3.894	13.052	-7.476	1.00	40.90	B
ATOM	3388	NH2	ARG	B	73	2.549	11.711	-8.772	1.00	41.65	B
ATOM	3389	C	ARG	B	73	3.074	17.695	-10.292	1.00	12.85	B
ATOM	3390	O	ARG	B	73	3.480	16.668	-10.851	1.00	12.28	B
ATOM	3391	N	LYS	B	74	2.530	18.708	-10.956	1.00	12.56	B
ATOM	3392	CA	LYS	B	74	2.387	18.655	-12.419	1.00	12.58	B
ATOM	3393	CB	LYS	B	74	1.647	19.886	-12.933	1.00	11.93	B
ATOM	3394	CG	LYS	B	74	0.149	19.815	-12.596	1.00	13.85	B
ATOM	3395	CD	LYS	B	74	-0.493	21.183	-12.811	1.00	15.33	B
ATOM	3396	CE	LYS	B	74	-1.982	21.112	-12.597	1.00	16.90	B
ATOM	3397	NZ	LYS	B	74	-2.482	22.535	-12.538	1.00	17.31	B
ATOM	3398	C	LYS	B	74	3.729	18.561	-13.101	1.00	11.10	B
ATOM	3399	O	LYS	B	74	3.882	17.738	-14.009	1.00	11.83	B
ATOM	3400	N	PHE	B	75	4.687	19.379	-12.673	1.00	11.16	B
ATOM	3401	CA	PHE	B	75	6.015	19.357	-13.326	1.00	8.77	B
ATOM	3402	CB	PHE	B	75	6.851	20.553	-12.866	1.00	9.59	B
ATOM	3403	CG	PHE	B	75	8.199	20.686	-13.568	1.00	11.61	B
ATOM	3404	CD1	PHE	B	75	8.300	20.587	-14.956	1.00	12.29	B
ATOM	3405	CD2	PHE	B	75	9.320	20.975	-12.835	1.00	12.93	B
ATOM	3406	CE1	PHE	B	75	9.567	20.782	-15.596	1.00	14.18	B
ATOM	3407	CE2	PHE	B	75	10.561	21.172	-13.448	1.00	16.28	B
ATOM	3408	CZ	PHE	B	75	10.677	21.069	-14.836	1.00	13.85	B
ATOM	3409	C	PHE	B	75	6.699	18.029	-13.066	1.00	10.84	B
ATOM	3410	O	PHE	B	75	7.225	17.420	-14.009	1.00	9.16	B
ATOM	3411	N	PHE	B	76	6.663	17.552	-11.819	1.00	10.39	B
ATOM	3412	CA	PHE	B	76	7.252	16.230	-11.555	1.00	11.16	B
ATOM	3413	CB	PHE	B	76	7.138	15.862	-10.092	1.00	12.23	B
ATOM	3414	CG	PHE	B	76	7.546	14.459	-9.823	1.00	14.40	B
ATOM	3415	CD1	PHE	B	76	8.888	14.117	-9.730	1.00	16.66	B
ATOM	3416	CD2	PHE	B	76	6.583	13.475	-9.667	1.00	16.99	B
ATOM	3417	CE1	PHE	B	76	9.252	12.795	-9.461	1.00	17.02	B
ATOM	3418	CE2	PHE	B	76	6.946	12.143	-9.407	1.00	17.99	B
ATOM	3419	CZ	PHE	B	76	8.275	11.821	-9.302	1.00	18.48	B
ATOM	3420	C	PHE	B	76	6.579	15.133	-12.373	1.00	12.82	B
ATOM	3421	O	PHE	B	76	7.255	14.307	-12.999	1.00	10.50	B
ATOM	3422	N	ASP	B	77	5.247	15.103	-12.399	1.00	10.55	B
ATOM	3423	CA	ASP	B	77	4.563	14.074	-13.173	1.00	9.78	B
ATOM	3424	CB	ASP	B	77	3.053	14.178	-12.970	1.00	11.78	B
ATOM	3425	CG	ASP	B	77	2.626	13.732	-11.596	1.00	17.39	B
ATOM	3426	OD1	ASP	B	77	3.439	13.121	-10.843	1.00	17.35	B
ATOM	3427	OD2	ASP	B	77	1.441	13.973	-11.260	1.00	18.13	B
ATOM	3428	C	ASP	B	77	4.893	14.113	-14.663	1.00	8.50	B
ATOM	3429	O	ASP	B	77	5.004	13.055	-15.288	1.00	10.06	B
ATOM	3430	N	ILE	B	78	5.065	15.316	-15.218	1.00	9.33	B
ATOM	3431	CA	ILE	B	78	5.427	15.449	-16.628	1.00	9.86	B
ATOM	3432	CB	ILE	B	78	5.451	16.940	-17.049	1.00	11.48	B
ATOM	3433	CG2	ILE	B	78	6.191	17.139	-18.424	1.00	13.90	B
ATOM	3434	CG1	ILE	B	78	3.976	17.389	-17.151	1.00	13.19	B
ATOM	3435	CD1	ILE	B	78	3.776	18.939	-17.260	1.00	16.24	B
ATOM	3436	C	ILE	B	78	6.817	14.832	-16.839	1.00	9.23	B
ATOM	3437	O	ILE	B	78	6.993	13.993	-17.726	1.00	10.91	B
ATOM	3438	N	CYS	B	79	7.762	15.226	-16.013	1.00	10.15	B
ATOM	3439	CA	CYS	B	79	9.131	14.699	-16.223	1.00	10.57	B
ATOM	3440	CB	CYS	B	79	10.081	15.403	-15.269	1.00	10.45	B
ATOM	3441	SG	CYS	B	79	10.273	17.176	-15.649	1.00	15.50	B
ATOM	3442	C	CYS	B	79	9.176	13.190	-16.024	1.00	12.39	B
ATOM	3443	O	CYS	B	79	9.819	12.455	-16.788	1.00	13.55	B
ATOM	3444	N	ARG	B	80	8.500	12.725	-14.982	1.00	10.64	B
ATOM	3445	CA	ARG	B	80	8.491	11.273	-14.719	1.00	12.98	B
ATOM	3446	CB	ARG	B	80	7.744	11.007	-13.399	1.00	15.52	B
ATOM	3447	CG	ARG	B	80	7.791	9.534	-12.911	1.00	20.13	B
ATOM	3448	CD	ARG	B	80	6.843	9.325	-11.713	1.00	25.38	B
ATOM	3449	NE	ARG	B	80	5.482	9.714	-12.093	1.00	31.58	B
ATOM	3450	CZ	ARG	B	80	4.456	9.888	-11.254	1.00	33.35	B
ATOM	3451	NH1	ARG	B	80	4.598	9.704	-9.939	1.00	35.49	B
ATOM	3452	NH2	ARG	B	80	3.280	10.257	-11.732	1.00	34.33	B
ATOM	3453	C	ARG	B	80	7.819	10.507	-15.846	1.00	13.18	B
ATOM	3454	O	ARG	B	80	8.159	9.360	-16.140	1.00	13.55	B
ATOM	3455	N	GLY	B	81	6.836	11.128	-16.484	1.00	11.84	B
ATOM	3456	CA	GLY	B	81	6.116	10.437	-17.522	1.00	11.90	B
ATOM	3457	C	GLY	B	81	6.781	10.356	-18.869	1.00	11.01	B
ATOM	3458	O	GLY	B	81	6.335	9.605	-19.734	1.00	11.50	B
ATOM	3459	N	LEU	B	82	7.806	11.188	-19.071	1.00	11.31	B
ATOM	3460	CA	LEU	B	82	8.514	11.169	-20.328	1.00	9.84	B
ATOM	3461	CB	LEU	B	82	9.370	12.430	-20.446	1.00	8.66	B
ATOM	3462	CG	LEU	B	82	8.522	13.680	-20.801	1.00	9.38	B
ATOM	3463	CD1	LEU	B	82	9.372	14.967	-20.574	1.00	9.37	B
ATOM	3464	CD2	LEU	B	82	8.050	13.551	-22.262	1.00	11.14	B
ATOM	3465	C	LEU	B	82	9.376	9.916	-20.380	1.00	11.17	B

Figure 1 (continued 35)

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ATOM   3466  O    LEU B  82      9.726    9.344  -19.347  1.00  12.58           B
ATOM   3467  N    PRO B  83      9.758    9.523  -21.590  1.00  11.69           B
ATOM   3468  CD   PRO B  83      9.531   10.208  -22.863  1.00  13.36           B
ATOM   3469  CA   PRO B  83     10.575    8.309  -21.770  1.00  12.94           B
ATOM   3470  CB   PRO B  83     10.597    8.140  -23.290  1.00  15.08           B
ATOM   3471  CG   PRO B  83     10.505    9.493  -23.806  1.00  14.86           B
ATOM   3472  C    PRO B  83     11.964    8.393  -21.150  1.00  15.17           B
ATOM   3473  O    PRO B  83     12.542    9.473  -21.023  1.00  14.86           B
ATOM   3474  N    GLU B  84     12.495    7.237  -20.759  1.00  15.45           B
ATOM   3475  CA   GLU B  84     13.817    7.220  -20.152  1.00  15.30           B
ATOM   3476  CB   GLU B  84     14.193    5.761  -19.825  1.00  17.19           B
ATOM   3477  CG   GLU B  84     15.507    5.588  -19.128  1.00  20.25           B
ATOM   3478  CD   GLU B  84     15.564    4.266  -18.419  1.00  22.78           B
ATOM   3479  OE1  GLU B  84     14.981    3.297  -18.955  1.00  27.86           B
ATOM   3480  OE2  GLU B  84     16.180    4.197  -17.344  1.00  25.77           B
ATOM   3481  C    GLU B  84     14.831    7.848  -21.116  1.00  13.55           B
ATOM   3482  O    GLU B  84     14.815    7.576  -22.325  1.00  16.08           B
ATOM   3483  N    GLY B  85     15.682    8.719  -20.573  1.00  15.12           B
ATOM   3484  CA   GLY B  85     16.714    9.359  -21.386  1.00  15.70           B
ATOM   3485  C    GLY B  85     16.279   10.612  -22.136  1.00  16.21           B
ATOM   3486  O    GLY B  85     17.088   11.268  -22.797  1.00  17.94           B
ATOM   3487  N    ALA B  86     14.995   10.955  -22.013  1.00  13.60           B
ATOM   3488  CA   ALA B  86     14.450   12.128  -22.688  1.00  13.37           B
ATOM   3489  CB   ALA B  86     12.944   12.293  -22.330  1.00  15.70           B
ATOM   3490  C    ALA B  86     15.161   13.416  -22.324  1.00  12.98           B
ATOM   3491  O    ALA B  86     15.551   13.631  -21.183  1.00  13.52           B
ATOM   3492  N    GLU B  87     15.341   14.285  -23.316  1.00  12.60           B
ATOM   3493  CA   GLU B  87     15.926   15.594  -23.086  1.00  12.20           B
ATOM   3494  CB   GLU B  87     16.650   16.050  -24.339  1.00  16.46           B
ATOM   3495  CG   GLU B  87     17.818   15.137  -24.688  1.00  20.50           B
ATOM   3496  CD   GLU B  87     18.945   15.208  -23.669  1.00  24.25           B
ATOM   3497  OE1  GLU B  87     18.958   16.145  -22.844  1.00  21.60           B
ATOM   3498  OE2  GLU B  87     19.827   14.308  -23.718  1.00  25.73           B
ATOM   3499  C    GLU B  87     14.734   16.512  -22.814  1.00  12.64           B
ATOM   3500  O    GLU B  87     13.810   16.527  -23.623  1.00  15.78           B
ATOM   3501  N    ILE B  88     14.770   17.241  -21.707  1.00  12.08           B
ATOM   3502  CA   ILE B  88     13.645   18.127  -21.325  1.00  11.17           B
ATOM   3503  CB   ILE B  88     13.218   17.788  -19.878  1.00  11.48           B
ATOM   3504  CG2  ILE B  88     11.990   18.637  -19.452  1.00  12.56           B
ATOM   3505  CG1  ILE B  88     12.887   16.294  -19.815  1.00  12.51           B
ATOM   3506  CD1  ILE B  88     12.482   15.794  -18.471  1.00  11.91           B
ATOM   3507  C    ILE B  88     14.067   19.573  -21.468  1.00  10.83           B
ATOM   3508  O    ILE B  88     14.909   20.066  -20.691  1.00  12.26           B
ATOM   3509  N    ALA B  89     13.477   20.261  -22.448  1.00  10.23           B
ATOM   3510  CA   ALA B  89     13.802   21.659  -22.723  1.00  10.42           B
ATOM   3511  CB   ALA B  89     13.784   21.911  -24.227  1.00  11.36           B
ATOM   3512  C    ALA B  89     12.738   22.517  -22.046  1.00  11.07           B
ATOM   3513  O    ALA B  89     11.542   22.297  -22.226  1.00  12.01           B
ATOM   3514  N    VAL B  90     13.196   23.508  -21.307  1.00  10.02           B
ATOM   3515  CA   VAL B  90     12.301   24.367  -20.549  1.00   9.76           B
ATOM   3516  CB   VAL B  90     12.499   24.064  -19.045  1.00  10.85           B
ATOM   3517  CG1  VAL B  90     11.583   24.955  -18.217  1.00  12.19           B
ATOM   3518  CG2  VAL B  90     12.171   22.613  -18.750  1.00  11.27           B
ATOM   3519  C    VAL B  90     12.577   25.830  -20.791  1.00  11.53           B
ATOM   3520  O    VAL B  90     13.731   26.256  -20.768  1.00  13.48           B
ATOM   3521  N    GLN B  91     11.523   26.617  -21.015  1.00  11.55           B
ATOM   3522  CA   GLN B  91     11.705   28.051  -21.210  1.00  14.62           B
ATOM   3523  CB   GLN B  91     11.889   28.401  -22.692  1.00  18.48           B
ATOM   3524  CG   GLN B  91     12.135   29.913  -22.891  1.00  26.33           B
ATOM   3525  CD   GLN B  91     12.980   30.211  -24.112  1.00  29.12           B
ATOM   3526  OE1  GLN B  91     13.538   31.308  -24.238  1.00  34.56           B
ATOM   3527  NE2  GLN B  91     13.073   29.248  -25.024  1.00  31.87           B
ATOM   3528  C    GLN B  91     10.550   28.838  -20.631  1.00  14.08           B
ATOM   3529  O    GLN B  91      9.367   28.487  -20.811  1.00  13.76           B
ATOM   3530  N    LEU B  92     10.908   29.885  -19.884  1.00  14.73           B
ATOM   3531  CA   LEU B  92      9.928   30.771  -19.267  1.00  15.30           B
ATOM   3532  CB   LEU B  92     10.575   31.606  -18.144  1.00  16.00           B
ATOM   3533  CG   LEU B  92      9.626   32.613  -17.459  1.00  15.51           B
ATOM   3534  CD1  LEU B  92      8.460   31.882  -16.765  1.00  18.05          ,B
ATOM   3535  CD2  LEU B  92     10.387   33.405  -16.426  1.00  17.67          !B
ATOM   3536  C    LEU B  92      9.435   31.694  -20.368  1.00  16.50           B
ATOM   3537  O    LEU B  92     10.259   32.293  -21.102  1.00  17.36           B
ATOM   3538  N    GLU B  93      8.107   31.790  -20.487  1.00  17.70           B
ATOM   3539  CA   GLU B  93      7.456   32.645  -21.469  1.00  20.10           B
ATOM   3540  CB   GLU B  93      6.889   31.788  -22.615  1.00  19.07           B
ATOM   3541  CG   GLU B  93      8.021   30.998  -23.341  1.00  20.16           B
ATOM   3542  CD   GLU B  93      7.622   30.371  -24.678  1.00  21.44           B
ATOM   3543  OE1  GLU B  93      6.413   30.147  -24.893  1.00  22.08           B
ATOM   3544  OE2  GLU B  93      8.530   30.087  -25.504  1.00  20.59           B
ATOM   3545  C    GLU B  93     -6.358  -33.451  -20.767  1.00  21.41           B
ATOM   3546  O    GLU B  93      5.165   33.286  -21.039  1.00  22.54           B
ATOM   3547  N    GLY B  94      6.774   34.296  -19.821  1.00  23.49           B
ATOM   3548  CA   GLY B  94      5.826   35.136  -19.099  1.00  23.13           B
ATOM   3549  C    GLY B  94      4.835   34.435  -18.182  1.00  23.80           B
ATOM   3550  O    GLY B  94      5.205   33.923  -17.126  1.00  23.56           B
ATOM   3551  N    GLU B  95      3.569   34.428  -18.574  1.00  21.90           B
ATOM   3552  CA   GLU B  95      2.539   33.797  -17.756  1.00  22.03           B
ATOM   3553  CB   GLU B  95      1.135   34.201  -18.269  1.00  25.70           B
ATOM   3554  CG   GLU B  95      0.715   33.489  -19.565  1.00  32.06           B
ATOM   3555  CD   GLU B  95     -0.577   34.015  -20.188  1.00  34.90           B
ATOM   3556  OE1  GLU B  95     -1.491   34.428  -19.437  1.00  35.44           B
ATOM   3557  OE2  GLU B  95     -0.679   33.994  -21.442  1.00  37.09           B
ATOM   3558  C    GLU B  95      2.680   32.262  -17.760  1.00  20.12           B
ATOM   3559  O    GLU B  95      2.076   31.573  -16.932  1.00  19.55           B
ATOM   3560  N    ARG B  96      3.465   31.726  -18.694  1.00  17.37           B
ATOM   3561  CA   ARG B  96      3.605   30.271  -18.751  1.00  14.55           B
ATOM   3562  CB   ARG B  96      2.777   29.683  -19.912  1.00  16.86           B
ATOM   3563  CG   ARG B  96      3.296   29.992  -21.341  1.00  16.89           B
ATOM   3564  CD   ARG B  96      4.258   28.903  -21.876  1.00  20.34           B
ATOM   3565  NE   ARG B  96      4.551   28.994  -23.319  1.00  22.54           B
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Figure 1 (continued 36)

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ATOM   3566  CZ   ARG B  96      3.842  28.445 -24.308  1.00 25.11           B
ATOM   3567  NH1  ARG B  96      2.742  27.746 -24.054  1.00 24.38           B
ATOM   3568  NH2  ARG B  96      4.276  28.546 -25.577  1.00 20.68           B
ATOM   3569  C    ARG B  96      5.025  29.829 -18.904  1.00 13.94           B
ATOM   3570  O    ARG B  96      5.883  30.602 -19.331  1.00 14.85           B
ATOM   3571  N    MET B  97      5.266  28.578 -18.520  1.00 12.30           B
ATOM   3572  CA   MET B  97      6.582  27.961 -18.667  1.00 10.91           B
ATOM   3573  CB   MET B  97      7.093  27.392 -17.326  1.00 10.86           B
ATOM   3574  CG   MET B  97      8.503  26.885 -17.487  1.00 14.36           B
ATOM   3575  SD   MET B  97      9.268  26.288 -15.952  1.00 14.09           B
ATOM   3576  CE   MET B  97      8.674  24.617 -15.920  1.00 15.27           B
ATOM   3577  C    MET B  97      6.336  26.817 -19.641  1.00 11.29           B
ATOM   3578  O    MET B  97      5.493  25.956 -19.386  1.00 11.55           B
ATOM   3579  N    LEU B  98      7.099  26.798 -20.750  1.00 10.37           B
ATOM   3580  CA   LEU B  98      6.935  25.818 -21.793  1.00  9.09           B
ATOM   3581  CB   LEU B  98      7.140  26.502 -23.145  1.00 10.04           B
ATOM   3582  CG   LEU B  98      7.119  25.556 -24.343  1.00 13.03           B
ATOM   3583  CD1  LEU B  98      5.756  24.875 -24.484  1.00 14.58           B
ATOM   3584  CD2  LEU B  98      7.499  26.390 -25.593  1.00 15.51           B
ATOM   3585  C    LEU B  98      7.936  24.703 -21.615  1.00 10.17           B
ATOM   3586  O    LEU B  98      9.121  24.991 -21.439  1.00 12.00           B
ATOM   3587  N    VAL B  99      7.440  23.469 -21.569  1.00  8.14           B
ATOM   3588  CA   VAL B  99      8.303  22.284 -21.423  1.00  9.99           B
ATOM   3589  CB   VAL B  99      7.831  21.408 -20.182  1.00  8.49           B
ATOM   3590  CG1  VAL B  99      8.712  20.156 -20.085  1.00 12.22           B
ATOM   3591  CG2  VAL B  99      7.813  22.225 -18.916  1.00 10.21           B
ATOM   3592  C    VAL B  99      8.169  21.454 -22.700  1.00 11.04           B
ATOM   3593  O    VAL B  99      7.031  21.087 -23.108  1.00 10.88           B
ATOM   3594  N    ARG B 100      9.293  21.137 -23.366  1.00  8.40           B
ATOM   3595  CA   ARG B 100      9.218  20.358 -24.593  1.00  8.30           B
ATOM   3596  CB   ARG B 100      9.613  21.220 -25.829  1.00 10.50           B
ATOM   3597  CG   ARG B 100      8.754  22.464 -26.057  1.00 11.28           B
ATOM   3598  CD   ARG B 100      9.404  23.363 -27.152  1.00 15.41           B
ATOM   3599  NE   ARG B 100     10.676  23.920 -26.707  1.00 16.70           B
ATOM   3600  CZ   ARG B 100     11.829  23.803 -27.375  1.00 17.28           B
ATOM   3601  NH1  ARG B 100     11.889  23.144 -28.526  1.00 21.89           B
ATOM   3602  NH2  ARG B 100     12.927  24.341 -26.876  1.00 22.39           B
ATOM   3603  C    ARG B 100     10.176  19.198 -24.523  1.00  9.77           B
ATOM   3604  O    ARG B 100     11.283  19.325 -23.982  1.00  9.86           B
ATOM   3605  N    SER B 101      9.725  18.074 -25.051  1.00  7.91           B
ATOM   3606  CA   SER B 101     10.578  16.881 -25.125  1.00 10.45           B
ATOM   3607  CB   SER B 101     10.549  16.126 -23.787  1.00 10.43           B
ATOM   3608  OG   SER B 101     11.462  14.998 -23.840  1.00 13.17           B
ATOM   3609  C    SER B 101     10.043  16.057 -26.265  1.00 12.22           B
ATOM   3610  O    SER B 101      8.875  15.686 -26.263  1.00 11.21           B
ATOM   3611  N    GLY B 102     10.900  15.720 -27.235  1.00 11.77           B
ATOM   3612  CA   GLY B 102     10.396  14.967 -28.376  1.00 11.79           B
ATOM   3613  C    GLY B 102      9.269  15.772 -29.010  1.00 11.95           B
ATOM   3614  O    GLY B 102      9.440  16.944 -29.277  1.00 13.86           B
ATOM   3615  N    ARG B 103      8.113  15.137 -29.248  1.00 13.24           B
ATOM   3616  CA   ARG B 103      6.950  15.842 -29.786  1.00 13.56           B
ATOM   3617  CB   ARG B 103      6.404  15.140 -31.024  1.00 15.71           B
ATOM   3618  CG   ARG B 103      7.403  15.240 -32.172  1.00 18.07           B
ATOM   3619  CD   ARG B 103      6.753  14.857 -33.491  1.00 20.42           B
ATOM   3620  NE   ARG B 103      6.426  13.446 -33.518  1.00 21.82           B
ATOM   3621  CZ   ARG B 103      5.798  12.861 -34.539  1.00 24.65           B
ATOM   3622  NH1  ARG B 103      5.437  13.580 -35.598  1.00 24.54           B
ATOM   3623  NH2  ARG B 103      5.564  11.560 -34.517  1.00 25.63           B
ATOM   3624  C    ARG B 103      5.893  15.933 -28.697  1.00 13.10           B
ATOM   3625  O    ARG B 103      4.685  15.809 -28.966  1.00 14.85           B
ATOM   3626  N    SER B 104      6.372  16.100 -27.468  1.00 10.09           B
ATOM   3627  CA   SER B 104      5.503  16.309 -26.293  1.00 11.86           B
ATOM   3628  CB   SER B 104      5.888  15.378 -25.138  1.00 12.18           B
ATOM   3629  OG   SER B 104      5.938  14.020 -25.597  1.00 12.05           B
ATOM   3630  C    SER B 104      5.701  17.775 -25.877  1.00 12.30           B
ATOM   3631  O    SER B 104      6.849  18.298 -25.815  1.00 12.26           B
ATOM   3632  N    ARG B 105      4.587  18.470 -25.625  1.00 10.81           B
ATOM   3633  CA   ARG B 105      4.659  19.867 -25.234  1.00 10.24           B
ATOM   3634  CB   ARG B 105      4.158  20.772 -26.370  1.00 12.01           B
ATOM   3635  CG   ARG B 105      5.004  20.788 -27.618  1.00 12.34           B
ATOM   3636  CD   ARG B 105      4.285  21.560 -28.760  1.00 13.57           B
ATOM   3637  NE   ARG B 105      3.799  22.896 -28.364  1.00 13.32           B
ATOM   3638  CZ   ARG B 105      4.552  23.991 -28.366  1.00 14.90           B
ATOM   3639  NH1  ARG B 105      5.822  23.903 -28.740  1.00 13.50           B
ATOM   3640  NH2  ARG B 105      4.037  25.165 -28.014  1.00 14.92           B
ATOM   3641  C    ARG B 105      3.757  20.122 -24.052  1.00  9.77           B
ATOM   3642  O    ARG B 105      2.639  19.588 -24.006  1.00 11.33           B
ATOM   3643  N    PHE B 106      4.221  20.929 -23.108  1.00 10.77           B
ATOM   3644  CA   PHE B 106      3.380  21.252 -21.939  1.00  9.20           B
ATOM   3645  CB   PHE B 106      3.795  20.410 -20.719  1.00 10.28           B
ATOM   3646  CG   PHE B 106      3.876  18.955 -21.000  1.00  9.68           B
ATOM   3647  CD1  PHE B 106      5.019  18.433 -21.591  1.00 12.41           B
ATOM   3648  CD2  PHE B 106      2.775  18.115 -20.793  1.00 12.06           B
ATOM   3649  CE1  PHE B 106      5.072  17.120 -21.982  1.00 12.35           B
ATOM   3650  CE2  PHE B 106      2.812  16.797 -21.182  1.00 13.89           B
ATOM   3651  CZ   PHE B 106      3.953  16.280 -21.783  1.00 14.71           B
ATOM   3652  C    PHE B 106      3.525  22.714 -21.579  1.00 12.00           B
ATOM   3653  O    PHE B 106      4.649  23.241 -21.528  1.00 11.63           B
ATOM   3654  N    SER B 107      2.389  23.375 -21.291  1.00 10.03           B
ATOM   3655  CA   SER B 107      2.415  24.766 -20.896  1.00 13.00           B
ATOM   3656  CB   SER B 107      1.559  25.595 -21.848  1.00 13.92           B
ATOM   3657  OG   SER B 107      1.547  26.962 -21.475  1.00 17.21           B
ATOM   3658  C    SER B 107      1.897  24.858 -19.471  1.00 13.30           B
ATOM   3659  O    SER B 107      0.741  24.542 -19.219  1.00 13.25           B
ATOM   3660  N    LEU B 108      2.774  25.213 -18.543  1.00 11.97           B
ATOM   3661  CA   LEU B 108      2.399  25.325 -17.130  1.00 12.30           B
ATOM   3662  CB   LEU B 108      3.497  24.741 -16.221  1.00 13.26           B
ATOM   3663  CG   LEU B 108      3.715  23.249 -16.427  1.00 15.24           B
ATOM   3664  CD1  LEU B 108      4.883  22.751 -15.567  1.00 14.96           B
ATOM   3665  CD2  LEU B 108      2.441  22.561 -16.079  1.00 15.65           B
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Figure 1 (continued 37)

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ATOM   3666  C    LEU B 108    2.210  26.768 -15.703  1.00 12.13      B
ATOM   3667  O    LEU B 108    2.936  27.647 -17.149  1.00 12.73      B
ATOM   3668  N    SER B 109    1.249  27.021 -15.807  1.00 13.50      B
ATOM   3669  CA   SER B 109    1.036  28.382 -15.313  1.00 15.61      B
ATOM   3670  CB   SER B 109   -0.345  28.466 -14.642  1.00 17.76      B
ATOM   3671  OG   SER B 109   -0.427  27.508 -13.599  1.00 25.01      B
ATOM   3672  C    SER B 109    2.118  28.695 -14.290  1.00 15.55      B
ATOM   3673  O    SER B 109    2.547  27.799 -13.536  1.00 18.85      B
ATOM   3674  N    THR B 110    2.550  29.935 -14.259  1.00 13.95      B
ATOM   3675  CA   THR B 110    3.587  30.367 -13.332  1.00 14.07      B
ATOM   3676  CB   THR B 110    4.749  31.074 -14.088  1.00 15.61      B
ATOM   3677  OG1  THR B 110    4.262  32.260 -14.719  1.00 16.22      B
ATOM   3678  CG2  THR B 110    5.333  30.173 -15.168  1.00 13.87      B
ATOM   3679  C    THR B 110    3.081  31.376 -12.323  1.00 14.62      B
ATOM   3680  O    THR B 110    2.028  32.023 -12.521  1.00 16.48      B
ATOM   3681  N    LEU B 111    3.835  31.498 -11.234  1.00 14.53      B
ATOM   3682  CA   LEU B 111    3.626  32.540 -10.236  1.00 14.82      B
ATOM   3683  CB   LEU B 111    3.048  31.999  -8.916  1.00 15.27      B
ATOM   3684  CG   LEU B 111    1.577  31.535  -8.991  1.00 16.13      B
ATOM   3685  CD1  LEU B 111    1.177  30.854  -7.706  1.00 15.76      B
ATOM   3686  CD2  LEU B 111    0.650  32.769  -9.243  1.00 15.24      B
ATOM   3687  C    LEU B 111    5.047  33.114 -10.070  1.00 16.26      B
ATOM   3688  O    LEU B 111    6.064  32.403 -10.174  1.00 16.00      B
ATOM   3689  N    PRO B 112    5.158  34.428  -9.873  1.00 15.54      B
ATOM   3690  CD   PRO B 112    4.031  35.374  -9.725  1.00 18.98      B
ATOM   3691  CA   PRO B 112    6.430  35.129  -9.711  1.00 16.92      B
ATOM   3692  CB   PRO B 112    5.984  36.546  -9.325  1.00 17.38      B
ATOM   3693  CG   PRO B 112    4.697  36.676 -10.033  1.00 19.99      B
ATOM   3694  C    PRO B 112    7.388  34.571  -8.674  1.00 15.89      B
ATOM   3695  O    PRO B 112    6.978  34.259  -7.552  1.00 17.87      B
ATOM   3696  N    ALA B 113    8.654  34.451  -9.066  1.00 17.65      B
ATOM   3697  CA   ALA B 113    9.702  33.993  -8.159  1.00 17.75      B
ATOM   3698  CB   ALA B 113   11.050  33.908  -8.901  1.00 18.59      B
ATOM   3699  C    ALA B 113    9.794  35.003  -6.997  1.00 19.95      B
ATOM   3700  O    ALA B 113   10.098  34.604  -5.873  1.00 18.56      B
ATOM   3701  N    ALA B 114    9.494  36.285  -7.254  1.00 19.88      B
ATOM   3702  CA   ALA B 114    9.546  37.297  -6.190  1.00 22.97      B
ATOM   3703  CB   ALA B 114    9.274  38.686  -6.762  1.00 24.68      B
ATOM   3704  C    ALA B 114    8.551  37.025  -5.073  1.00 24.13      B
ATOM   3705  O    ALA B 114    8.735  37.506  -3.948  1.00 25.27      B
ATOM   3706  N    ASP B 115    7.499  36.270  -5.374  1.00 22.97      B
ATOM   3707  CA   ASP B 115    6.458  35.936  -4.398  1.00 21.92      B
ATOM   3708  CB   ASP B 115    5.095  35.838  -5.085  1.00 25.25      B
ATOM   3709  CG   ASP B 115    4.653  37.144  -5.702  1.00 27.35      B
ATOM   3710  OD1  ASP B 115    5.197  38.200  -5.325  1.00 32.10      B
ATOM   3711  OD2  ASP B 115    3.756  37.115  -6.562  1.00 30.15      B
ATOM   3712  C    ASP B 115    6.686  34.620  -3.639  1.00 20.39      B
ATOM   3713  O    ASP B 115    5.892  34.256  -2.770  1.00 19.74      B
ATOM   3714  N    PHE B 116    7.743  33.883  -3.987  1.00 17.71      B
ATOM   3715  CA   PHE B 116    7.987  32.602  -3.323  1.00 18.38      B
ATOM   3716  CB   PHE B 116    9.004  31.796  -4.157  1.00 17.21      B
ATOM   3717  CG   PHE B 116    9.043  30.332  -3.810  1.00 18.03      B
ATOM   3718  CD1  PHE B 116    8.071  29.452  -4.300  1.00 16.40      B
ATOM   3719  CD2  PHE B 116   10.026  29.837  -2.955  1.00 17.20      B
ATOM   3720  CE1  PHE B 116    8.072  28.104  -3.949  1.00 18.94      B
ATOM   3721  CE2  PHE B 116   10.029  28.479  -2.596  1.00 15.80      B
ATOM   3722  CZ   PHE B 116    9.057  27.613  -3.091  1.00 18.24      B
ATOM   3723  C    PHE B 116    8.510  32.836  -1.896  1.00 18.89      B
ATOM   3724  O    PHE B 116    9.449  33.594  -1.716  1.00 19.05      B
ATOM   3725  N    PRO B 117    7.914  32.172  -0.888  1.00 20.37      B
ATOM   3726  CD   PRO B 117    6.913  31.117  -1.080  1.00 20.82      B
ATOM   3727  CA   PRO B 117    8.284  32.285   0.535  1.00 22.94      B
ATOM   3728  CB   PRO B 117    7.397  31.244   1.226  1.00 24.98      B
ATOM   3729  CG   PRO B 117    6.285  30.991   0.290  1.00 22.83      B
ATOM   3730  C    PRO B 117    9.736  31.922   0.684  1.00 25.37      B
ATOM   3731  O    PRO B 117   10.204  31.012   0.018  1.00 26.02      B
ATOM   3732  N    ASN B 118   10.441  32.630   1.556  1.00 27.41      B
ATOM   3733  CA   ASN B 118   11.857  32.398   1.767  1.00 30.63      B
ATOM   3734  CB   ASN B 118   12.638  33.537   1.081  1.00 34.20      B
ATOM   3735  CG   ASN B 118   14.111  33.525   1.411  1.00 36.43      B
ATOM   3736  OD1  ASN B 118   14.518  33.929   2.500  1.00 39.71      B
ATOM   3737  ND2  ASN B 118   14.922  33.052   0.472  1.00 40.26      B
ATOM   3738  C    ASN B 118   12.103  32.399   3.275  1.00 31.98      B
ATOM   3739  O    ASN B 118   11.683  33.332   3.959  1.00 32.47      B
ATOM   3740  N    LEU B 119   12.746  31.365   3.810  1.00 31.29      B
ATOM   3741  CA   LEU B 119   13.013  31.372   5.242  1.00 32.34      B
ATOM   3742  CB   LEU B 119   13.616  30.042   5.713  1.00 32.40      B
ATOM   3743  CG   LEU B 119   12.712  28.820   5.889  1.00 32.42      B
ATOM   3744  CD1  LEU B 119   13.507  27.710   6.551  1.00 34.29      B
ATOM   3745  CD2  LEU B 119   11.516  29.170   6.758  1.00 30.06      B
ATOM   3746  C    LEU B 119   13.996  32.502   5.540  1.00 32.87      B
ATOM   3747  O    LEU B 119   14.922  32.751   4.767  1.00 32.78      B
ATOM   3748  N    ASP B 120   13.785  33.170   6.668  1.00 33.27      B
ATOM   3749  CA   ASP B 120   14.634  34.264   7.106  1.00 35.53      B
ATOM   3750  CB   ASP B 120   14.100  34.820   8.442  1.00 38.51      B
ATOM   3751  CG   ASP B 120   14.813  36.102   8.896  1.00 41.15      B
ATOM   3752  OD1  ASP B 120   15.288  36.880   8.032  1.00 42.97      B
ATOM   3753  OD2  ASP B 120   14.878  36.341  10.128  1.00 41.78      B
ATOM   3754  C    ASP B 120   16.076  33.793   7.240  1.00 34.92      B
ATOM   3755  O    ASP B 120   16.366  32.615   7.430  1.00 33.81      B
ATOM   3756  N    ASP B 121   16.984  34.737   7.103  1.00 34.47      B
ATOM   3757  CA   ASP B 121   18.393  34.466   7.212  1.00 33.96      B
ATOM   3758  CB   ASP B 121   19.125  35.724   6.770  1.00 38.12      B
ATOM   3759  CG   ASP B 121   18.471  36.339   5.540  1.00 41.54      B
ATOM   3760  OD1  ASP B 121   18.665  35.786   4.433  1.00 42.91      B
ATOM   3761  OD2  ASP B 121   17.730  37.344   5.687  1.00 44.40      B
ATOM   3762  C    ASP B 121   18.648  34.144   8.672  1.00 31.06      B
ATOM   3763  O    ASP B 121   17.935  34.611   9.549  1.00 30.33      B
ATOM   3764  N    TRP B 122   19.642  33.314   8.927  1.00 29.45      B
ATOM   3765  CA   TRP B 122   19.953  32.969  10.301  1.00 26.54      B
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Figure 1 (continued 38)

ATOM	3766	CB	TRP	B	122	19.021	31.833	10.766	1.00	24.27	B
ATOM	3767	CG	TRP	B	122	19.072	30.629	9.899	1.00	23.67	B
ATOM	3768	CD2	TRP	B	122	19.832	29.445	10.127	1.00	23.03	B
ATOM	3769	CE2	TRP	B	122	19.617	28.587	9.027	1.00	24.46	B
ATOM	3770	CE3	TRP	B	122	20.680	29.020	11.157	1.00	21.61	B
ATOM	3771	CD1	TRP	B	122	18.435	30.451	8.697	1.00	25.67	B
ATOM	3772	NE1	TRP	B	122	18.760	29.225	8.167	1.00	25.03	B
ATOM	3773	CZ2	TRP	B	122	20.224	27.327	8.929	1.00	24.86	B
ATOM	3774	CZ3	TRP	B	122	21.276	27.769	11.061	1.00	21.60	B
ATOM	3775	CH2	TRP	B	122	21.047	26.940	9.956	1.00	25.02	B
ATOM	3776	C	TRP	B	122	21.416	32.581	10.381	1.00	25.76	B
ATOM	3777	O	TRP	B	122	22.081	32.419	9.354	1.00	25.40	B
ATOM	3778	N	GLN	B	123	21.932	32.437	11.600	1.00	22.86	B
ATOM	3779	CA	GLN	B	123	23.330	32.106	11.786	1.00	25.29	B
ATOM	3780	CB	GLN	B	123	23.960	33.225	12.614	1.00	23.33	B
ATOM	3781	CG	GLN	B	123	23.736	34.611	12.017	1.00	28.45	B
ATOM	3782	CD	GLN	B	123	24.576	34.837	10.772	1.00	28.70	B
ATOM	3783	OE1	GLN	B	123	24.445	35.856	10.099	1.00	32.60	B
ATOM	3784	NE2	GLN	B	123	25.447	33.889	10.469	1.00	32.57	B
ATOM	3785	C	GLN	B	123	23.537	30.762	12.492	1.00	24.00	B
ATOM	3786	O	GLN	B	123	22.879	30.502	13.494	1.00	25.77	B
ATOM	3787	N	SER	B	124	24.440	29.917	11.994	1.00	23.58	B
ATOM	3788	CA	SER	B	124	24.680	28.643	12.680	1.00	24.40	B
ATOM	3789	CB	SER	B	124	25.295	27.574	11.778	1.00	26.13	B
ATOM	3790	OG	SER	B	124	26.636	27.883	11.441	1.00	32.13	B
ATOM	3791	C	SER	B	124	25.600	28.849	13.870	1.00	24.43	B
ATOM	3792	O	SER	B	124	26.566	29.622	13.803	1.00	24.71	B
ATOM	3793	N	GLU	B	125	25.274	28.155	14.952	1.00	23.06	B
ATOM	3794	CA	GLU	B	125	26.035	28.205	16.203	1.00	24.57	B
ATOM	3795	CB	GLU	B	125	25.093	28.516	17.360	1.00	25.73	B
ATOM	3796	CG	GLU	B	125	24.399	29.857	17.254	1.00	32.47	B
ATOM	3797	CD	GLU	B	125	23.353	30.051	18.344	1.00	35.90	B
ATOM	3798	OE1	GLU	B	125	23.423	29.345	19.381	1.00	39.08	B
ATOM	3799	OE2	GLU	B	125	22.464	30.912	18.168	1.00	39.18	B
ATOM	3800	C	GLU	B	125	26.786	26.907	16.508	1.00	24.50	B
ATOM	3801	O	GLU	B	125	27.665	26.879	17.382	1.00	24.43	B
ATOM	3802	N	VAL	B	126	26.419	25.815	15.844	1.00	22.81	B
ATOM	3803	CA	VAL	B	126	27.106	24.539	16.031	1.00	24.05	B
ATOM	3804	CB	VAL	B	126	26.434	23.637	17.119	1.00	24.27	B
ATOM	3805	CG1	VAL	B	126	25.027	23.339	16.751	1.00	25.14	B
ATOM	3806	CG2	VAL	B	126	27.216	22.320	17.271	1.00	27.01	B
ATOM	3807	C	VAL	B	126	27.078	23.835	14.690	1.00	23.78	B
ATOM	3808	O	VAL	B	126	26.073	23.885	13.967	1.00	24.92	B
ATOM	3809	N	GLU	B	127	28.182	23.193	14.344	1.00	22.15	B
ATOM	3810	CA	GLU	B	127	28.281	22.509	13.081	1.00	21.91	B
ATOM	3811	CB	GLU	B	127	39.002	23.394	12.051	1.00	23.10	B
ATOM	3812	CG	GLU	B	127	28.426	24.768	11.966	1.00	26.12	B
ATOM	3813	CD	GLU	B	127	29.056	25.636	10.884	1.00	27.63	B
ATOM	3814	OE1	GLU	B	127	28.434	26.672	10.546	1.00	27.53	B
ATOM	3815	OE2	GLU	B	127	30.157	25.298	10.403	1.00	28.31	B
ATOM	3816	C	GLU	B	127	29.069	21.240	13.254	1.00	21.48	B
ATOM	3817	O	GLU	B	127	30.034	21.189	14.027	1.00	22.56	B
ATOM	3818	N	PHE	B	128	28.665	20.215	12.536	1.00	20.20	B
ATOM	3819	CA	PHE	B	128	29.377	18.956	12.576	1.00	19.84	B
ATOM	3820	CB	PHE	B	128	29.096	18.211	13.895	1.00	21.34	B
ATOM	3821	CG	PHE	B	128	27.632	18.001	14.172	1.00	19.59	B
ATOM	3822	CD1	PHE	B	128	26.892	18.969	14.829	1.00	20.54	B
ATOM	3823	CD2	PHE	B	128	26.993	16.851	13.729	1.00	19.54	B
ATOM	3824	CE1	PHE	B	128	25.516	18.802	15.043	1.00	18.79	B
ATOM	3825	CE2	PHE	B	128	25.616	16.672	13.938	1.00	20.56	B
ATOM	3826	CZ	PHE	B	128	24.886	17.646	14.591	1.00	20.20	B
ATOM	3827	C	PHE	B	128	28.997	18.096	11.392	1.00	21.44	B
ATOM	3828	O	PHE	B	128	27.986	18.338	10.707	1.00	19.41	B
ATOM	3829	N	THR	B	129	29.836	17.110	11.111	1.00	19.99	B
ATOM	3830	CA	THR	B	129	29.562	16.198	10.029	1.00	22.84	B
ATOM	3831	CB	THR	B	129	30.712	16.238	8.982	1.00	25.69	B
ATOM	3832	OG1	THR	B	129	31.949	15.897	9.626	1.00	32.56	B
ATOM	3833	CG2	THR	B	129	30.846	17.633	8.404	1.00	25.73	B
ATOM	3834	C	THR	B	129	29.415	14.792	10.608	1.00	24.49	B
ATOM	3835	O	THR	B	129	30.021	14.476	11.630	1.00	26.37	B
ATOM	3836	N	LEU	B	130	28.577	13.964	10.000	1.00	24.49	B
ATOM	3837	CA	LEU	B	130	28.423	12.589	10.477	1.00	24.08	B
ATOM	3838	CB	LEU	B	130	27.407	12.505	11.633	1.00	25.54	B
ATOM	3839	CG	LEU	B	130	25.900	12.579	11.337	1.00	25.32	B
ATOM	3840	CD1	LEU	B	130	25.149	12.111	12.598	1.00	24.84	B
ATOM	3841	CD2	LEU	B	130	25.477	13.989	10.960	1.00	23.86	B
ATOM	3842	C	LEU	B	130	27.965	11.707	9.327	1.00	23.70	B
ATOM	3843	O	LEU	B	130	27.413	12.191	8.343	1.00	23.84	B
ATOM	3844	N	PRO	B	131	28.197	10.389	9.425	1.00	23.64	B
ATOM	3845	CD	PRO	B	131	28.932	9.700	10.501	1.00	22.59	B
ATOM	3846	CA	PRO	B	131	27.790	9.465	8.371	1.00	22.27	B
ATOM	3847	CB	PRO	B	131	28.311	8.105	8.871	1.00	23.69	B
ATOM	3848	CG	PRO	B	131	29.456	8.479	9.793	1.00	23.88	B
ATOM	3849	C	PRO	B	131	26.273	9.459	8.237	1.00	23.45	B
ATOM	3850	O	PRO	B	131	25.555	9.578	9.239	1.00	21.35	B
ATOM	3851	N	GLN	B	132	25.778	9.341	7.013	1.00	22.22	B
ATOM	3852	CA	GLN	B	132	24.337	9.290	6.833	1.00	24.38	B
ATOM	3853	CB	GLN	B	132	23.975	9.060	5.383	1.00	27.52	B
ATOM	3854	CG	GLN	B	132	24.306	10.174	4.466	1.00	30.36	B
ATOM	3855	CD	GLN	B	132	23.834	9.867	3.061	1.00	32.41	B
ATOM	3856	OE1	GLN	B	132	22.667	9.539	2.845	1.00	34.45	B
ATOM	3857	NE2	GLN	B	132	24.736	9.964	2.100	1.00	33.22	B
ATOM	3858	C	GLN	B	132	23.737	8.134	7.642	1.00	24.58	B
ATOM	3859	O	GLN	B	132	22.646	8.253	8.187	1.00	23.73	B
ATOM	3860	N	ALA	B	133	24.446	7.005	7.692	1.00	24.46	B
ATOM	3861	CA	ALA	B	133	23.940	5.844	8.416	1.00	23.74	B
ATOM	3862	CB	ALA	B	133	24.911	4.650	8.241	1.00	25.48	B
ATOM	3863	C	ALA	B	133	23.677	6.103	9.896	1.00	22.24	B
ATOM	3864	O	ALA	B	133	22.768	5.493	10.482	1.00	23.23	B
ATOM	3865	N	THR	B	134	24.470	6.976	10.498	1.00	21.71	B

Figure 1 (continued 39)

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ATOM   3866   CA    THR  B 134      24.329    7.337   11.906   1.00 21.35      B
ATOM   3867   CB    THR  B 134      25.520    8.155   12.368   1.00 23.54      B
ATOM   3868   OG1   THR  B 134      26.705    7.376   12.169   1.00 25.66      B
ATOM   3869   CG2   THR  B 134      25.375    8.570   13.812   1.00 22.93      B
ATOM   3870   C     THR  B 134      23.077    8.161   12.089   1.00 20.95      B
ATOM   3871   O     THR  B 134      22.329    7.988   13.053   1.00 20.93      B
ATOM   3872   N     MET  B 135      22.855    9.097   11.172   1.00 19.95      B
ATOM   3873   CA    MET  B 135      21.654    9.897   11.284   1.00 20.19      B
ATOM   3874   CB    MET  B 135      21.626   10.994   10.222   1.00 20.76      B
ATOM   3875   CG    MET  B 135      20.385   11.886   10.326   1.00 22.47      B
ATOM   3876   SD    MET  B 135      20.158   12.699   11.928   1.00 25.83      B
ATOM   3877   CE    MET  B 135      21.360   14.018   11.870   1.00 26.97      B
ATOM   3878   C     MET  B 135      20.442    8.986   11.114   1.00 18.60      B
ATOM   3879   O     MET  B 135      19.453    9.134   11.831   1.00 18.63      B
ATOM   3880   N     LYS  B 136      20.487    8.053   10.169   1.00 19.85      B
ATOM   3881   CA    LYS  B 136      19.356    7.155    9.976   1.00 21.55      B
ATOM   3882   CB    LYS  B 136      19.595    6.173    8.831   1.00 24.24      B
ATOM   3883   CG    LYS  B 136      18.382    5.263    8.598   1.00 25.85      B
ATOM   3884   CD    LYS  B 136      18.333    4.703    7.182   1.00 32.16      B
ATOM   3885   CE    LYS  B 136      19.291    3.541    7.025   1.00 33.18      B
ATOM   3886   NZ    LYS  B 136      18.863    2.381    7.861   1.00 36.66      B
ATOM   3887   C     LYS  B 136      19.092    6.348   11.249   1.00 22.36      B
ATOM   3888   O     LYS  B 136      17.957    6.211   11.685   1.00 21.54      B
ATOM   3889   N     ARG  B 137      20.154    5.791   11.819   1.00 21.72      B
ATOM   3890   CA    ARG  B 137      20.004    4.998   13.037   1.00 21.93      B
ATOM   3891   CB    ARG  B 137      21.368    4.481   13.501   1.00 24.73      B
ATOM   3892   CG    ARG  B 137      21.339    3.432   14.643   1.00 28.08      B
ATOM   3893   CD    ARG  B 137      21.297    4.069   16.012   1.00 30.79      B
ATOM   3894   NE    ARG  B 137      21.609    3.129   17.104   1.00 31.38      B
ATOM   3895   CZ    ARG  B 137      20.802    2.161   17.547   1.00 31.74      B
ATOM   3896   NH1   ARG  B 137      19.604    1.962   17.003   1.00 31.80      B
ATOM   3897   NH2   ARG  B 137      21.184    1.411   18.578   1.00 29.88      B
ATOM   3898   C     ARG  B 137      19.360    5.820   14.141   1.00 20.76      B
ATOM   3899   O     ARG  B 137      18.389    5.386   14.770   1.00 21.28      B
ATOM   3900   N     LEU  B 138      19.880    7.021   14.364   1.00 19.03      B
ATOM   3901   CA    LEU  B 138      19.355    7.902   15.415   1.00 17.43      B
ATOM   3902   CB    LEU  B 138      20.123    9.223   15.421   1.00 17.77      B
ATOM   3903   CG    LEU  B 138      21.500    9.129   16.066   1.00 18.25      B
ATOM   3904   CD1   LEU  B 138      22.325   10.379   15.773   1.00 18.28      B
ATOM   3905   CD2   LEU  B 138      21.330    8.948   17.581   1.00 18.59      B
ATOM   3906   C     LEU  B 138      17.875    8.209   15.283   1.00 19.04      B
ATOM   3907   O     LEU  B 138      17.130    8.236   16.291   1.00 17.18      B
ATOM   3908   N     ILE  B 139      17.436    8.467   14.055   1.00 16.38      B
ATOM   3909   CA    ILE  B 139      16.027    8.783   13.843   1.00 16.79      B
ATOM   3910   CB    ILE  B 139      15.811    9.516   12.479   1.00 16.68      B
ATOM   3911   CG2   ILE  B 139      14.322    9.634   12.168   1.00 20.18      B
ATOM   3912   CG1   ILE  B 139      16.478   10.883   12.561   1.00 18.34      B
ATOM   3913   CD1   ILE  B 139      16.478   11.689   11.221   1.00 19.90      B
ATOM   3914   C     ILE  B 139      15.143    7.553   13.916   1.00 16.56      B
ATOM   3915   O     ILE  B 139      14.128    7.563   14.590   1.00 16.80      B
ATOM   3916   N     GLU  B 140      15.526    6.482   13.238   1.00 15.42      B
ATOM   3917   CA    GLU  B 140      14.720    5.276   13.263   1.00 16.12      B
ATOM   3918   CB    GLU  B 140      15.316    4.232   12.322   1.00 17.99      B
ATOM   3919   CG    GLU  B 140      15.176    4.640   10.858   1.00 22.86      B
ATOM   3920   CD    GLU  B 140      15.372    3.489    9.890   1.00 27.30      B
ATOM   3921   OE1   GLU  B 140      16.289    2.678   10.103   1.00 28.72      B
ATOM   3922   OE2   GLU  B 140      14.609    3.402    8.905   1.00 31.19      B
ATOM   3923   C     GLU  B 140      14.595    4.687   14.676   1.00 15.11      B
ATOM   3924   O     GLU  B 140      13.591    4.042   15.003   1.00 17.70      B
ATOM   3925   N     ALA  B 141      15.609    4.903   15.503   1.00 15.65      B
ATOM   3926   CA    ALA  B 141      15.577    4.336   16.849   1.00 15.07      B
ATOM   3927   CB    ALA  B 141      16.963    4.469   17.487   1.00 18.37      B
ATOM   3928   C     ALA  B 141      14.530    5.000   17.751   1.00 14.92      B
ATOM   3929   O     ALA  B 141      14.080    4.409   18.734   1.00 14.51      B
ATOM   3930   N     THR  B 142      14.097    6.209   17.401   1.00 13.57      B
ATOM   3931   CA    THR  B 142      13.205    6.922   18.309   1.00 13.58      B
ATOM   3932   CB    THR  B 142      13.994    8.081   18.978   1.00 17.09      B
ATOM   3933   OG1   THR  B 142      14.329    9.057   17.962   1.00 17.94      B
ATOM   3934   CG2   THR  B 142      15.336    7.553   19.627   1.00 15.55      B
ATOM   3935   C     THR  B 142      11.943    7.507   17.706   1.00 14.63      B
ATOM   3936   O     THR  B 142      11.004    7.820   18.438   1.00 13.14      B
ATOM   3937   N     GLN  B 143      11.899    7.640   16.381   1.00 13.61      B
ATOM   3938   CA    GLN  B 143      10.752    8.313   15.743   1.00 15.74      B
ATOM   3939   CB    GLN  B 143      10.937    8.285   14.215   1.00 17.04      B
ATOM   3940   CG    GLN  B 143       9.799    8.931   13.418   1.00 18.95      B
ATOM   3941   CD    GLN  B 143      10.073    8.886   11.922   1.00 22.30      B
ATOM   3942   OE1   GLN  B 143      10.552    7.873   11.411   1.00 23.43      B
ATOM   3943   NE2   GLN  B 143       9.769    9.989   11.211   1.00 23.11      B
ATOM   3944   C     GLN  B 143       9.380    7.797   16.137   1.00 15.74      B
ATOM   3945   O     GLN  B 143       8.438    8.577   16.322   1.00 17.49      B
ATOM   3946   N     PHE  B 144       9.254    6.489   16.319   1.00 15.47      B
ATOM   3947   CA    PHE  B 144       7.951    5.942   16.640   1.00 15.79      B
ATOM   3948   CB    PHE  B 144       8.009    4.408   16.623   1.00 16.45      B
ATOM   3949   CG    PHE  B 144       8.745    3.818   17.785   1.00 15.61      B
ATOM   3950   CD1   PHE  B 144      10.129    3.644   17.740   1.00 14.87      B
ATOM   3951   CD2   PHE  B 144       8.052    3.490   18.952   1.00 15.49      B
ATOM   3952   CE1   PHE  B 144      10.825    3.158   18.849   1.00 14.78      B
ATOM   3953   CE2   PHE  B 144       8.730    3.002   20.072   1.00 14.34      B
ATOM   3954   CZ    PHE  B 144      10.108    2.836   20.033   1.00 15.36      B
ATOM   3955   C     PHE  B 144       7.390    6.402   17.979   1.00 16.39      B
ATOM   3956   O     PHE  B 144       6.196    6.252   18.206   1.00 16.31      B
ATOM   3957   N     SER  B 145       8.233    6.932   18.857   1.00 15.52      B
ATOM   3958   CA    SER  B 145       7.765    7.357   20.178   1.00 15.49      B
ATOM   3959   CB    SER  B 145       8.842    7.137   21.236   1.00 19.43      B
ATOM   3960   OG    SER  B 145       9.051    5.743   21.459   1.00 19.03      B
ATOM   3961   C     SER  B 145       7.321    8.812   20.231   1.00 17.97      B
ATOM   3962   O     SER  B 145       6.983    9.307   21.325   1.00 17.36      B
ATOM   3963   N     MET  B 146       7.362    9.507   19.093   1.00 17.94      B
ATOM   3964   CA    MET  B 146       6.910   10.907   19.066   1.00 19.19      B
ATOM   3965   CB    MET  B 146       7.260   11.560   17.711   1.00 21.36      B
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Figure 1 (continued 40)

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ATOM   3966  CG   MET B 146       8.716  11.608  17.434  1.00 19.66           B
ATOM   3967  SD   MET B 146       8.961  11.941  15.674  1.00 23.93           B
ATOM   3968  CE   MET B 146       8.838  13.621  15.659  1.00 23.07           B
ATOM   3969  C    MET B 146       5.393  10.948  19.237  1.00 19.89           B
ATOM   3970  O    MET B 146       4.683  10.038  18.798  1.00 21.24           B
ATOM   3971  N    ALA B 147       4.879  12.014  19.853  1.00 21.60           B
ATOM   3972  CA   ALA B 147       3.438  12.137  20.009  1.00 24.00           B
ATOM   3973  CB   ALA B 147       3.112  13.270  21.028  1.00 23.97           B
ATOM   3974  C    ALA B 147       2.775  12.439  18.661  1.00 25.73           B
ATOM   3975  O    ALA B 147       3.433  12.878  17.714  1.00 23.85           B
ATOM   3976  N    HIS B 148       1.473  12.184  18.568  1.00 30.66           B
ATOM   3977  CA   HIS B 148       0.719  12.469  17.348  1.00 34.48           B
ATOM   3978  CB   HIS B 148       0.020  11.211  16.829  1.00 37.35           B
ATOM   3979  CG   HIS B 148       0.944  10.060  16.595  1.00 40.57           B
ATOM   3980  CD2  HIS B 148       0.913   8.786  17.053  1.00 41.90           B
ATOM   3981  ND1  HIS B 148       2.056  10.150  15.783  1.00 42.40           B
ATOM   3982  CE1  HIS B 148       2.672   8.981  15.754  1.00 42.24           B
ATOM   3983  NE2  HIS B 148       1.998   8.136  16.515  1.00 43.11           B
ATOM   3984  C    HIS B 148      -0.344  13.519  17.668  1.00 36.54           B
ATOM   3985  O    HIS B 148      -1.386  13.201  18.262  1.00 36.38           B
ATOM   3986  N    GLN B 149      -0.078  14.761  17.281  1.00 37.77           B
ATOM   3987  CA   GLN B 149      -1.019  15.853  17.523  1.00 39.65           B
ATOM   3988  CB   GLN B 149      -2.290  15.638  16.680  1.00 41.57           B
ATOM   3989  CG   GLN B 149      -2.022  15.462  15.185  1.00 44.91           B
ATOM   3990  CD   GLN B 149      -3.278  15.215  14.355  1.00 46.65           B
ATOM   3991  OE1  GLN B 149      -4.068  14.320  14.648  1.00 48.28           B
ATOM   3992  NE2  GLN B 149      -3.453  16.003  13.300  1.00 48.05           B
ATOM   3993  C    GLN B 149      -1.376  15.995  19.005  1.00 39.02           B
ATOM   3994  O    GLN B 149      -2.558  16.067  19.370  1.00 40.48           B
ATOM   3995  N    ASP B 150      -0.354  16.029  19.857  1.00 38.46           B
ATOM   3996  CA   ASP B 150      -0.534  16.192  21.299  1.00 37.30           B
ATOM   3997  CB   ASP B 150       0.679  15.640  22.059  1.00 37.60           B
ATOM   3998  CG   ASP B 150       0.445  15.547  23.561  1.00 38.25           B
ATOM   3999  OD1  ASP B 150       0.093  16.575  24.172  1.00 38.49           B
ATOM   4000  OD2  ASP B 150       0.621  14.450  24.149  1.00 37.98           B
ATOM   4001  C    ASP B 150      -0.673  17.695  21.578  1.00 38.03           B
ATOM   4002  O    ASP B 150      -0.191  18.526  20.803  1.00 35.91           B
ATOM   4003  N    VAL B 151      -1.325  18.036  22.687  1.00 38.58           B
ATOM   4004  CA   VAL B 151      -1.527  19.432  23.055  1.00 38.83           B
ATOM   4005  CB   VAL B 151      -2.403  19.567  24.316  1.00 39.52           B
ATOM   4006  CG1  VAL B 151      -2.705  21.028  24.579  1.00 39.97           B
ATOM   4007  CG2  VAL B 151      -3.678  18.778  24.142  1.00 40.52           B
ATOM   4008  C    VAL B 151      -0.185  20.057  23.331  1.00 38.33           B
ATOM   4009  O    VAL B 151       0.047  21.213  22.982  1.00 38.42           B
ATOM   4010  N    ARG B 152       0.676  19.302  24.012  1.00 37.29           B
ATOM   4011  CA   ARG B 152       2.022  19.761  24.291  1.00 36.95           B
ATOM   4012  CB   ARG B 152       2.718  18.842  25.304  1.00 38.55           B
ATOM   4013  CG   ARG B 152       2.144  18.896  26.717  1.00 40.64           B
ATOM   4014  CD   ARG B 152       0.984  17.935  26.875  1.00 41.39           B
ATOM   4015  NE   ARG B 152       1.454  16.561  27.041  1.00 43.21           B
ATOM   4016  CZ   ARG B 152       0.674  15.492  26.935  1.00 44.44           B
ATOM   4017  NH1  ARG B 152      -0.619  15.645  26.656  1.00 46.42           B
ATOM   4018  NH2  ARG B 152       1.176  14.274  27.116  1.00 43.86           B
ATOM   4019  C    ARG B 152       2.683  19.626  22.921  1.00 36.41           B
ATOM   4020  O    ARG B 152       3.410  18.659  22.678  1.00 34.83           B
ATOM   4021  N    TYR B 153       2.403  20.580  22.031  1.00 34.80           B
ATOM   4022  CA   TYR B 153       2.927  20.555  20.665  1.00 33.74           B
ATOM   4023  CB   TYR B 153       2.686  21.906  19.963  1.00 35.98           B
ATOM   4024  CG   TYR B 153       3.406  23.061  20.611  1.00 38.54           B
ATOM   4025  CD1  TYR B 153       2.975  23.581  21.835  1.00 39.34           B
ATOM   4026  CE1  TYR B 153       3.698  24.581  22.487  1.00 39.67           B
ATOM   4027  CD2  TYR B 153       4.574  23.582  20.049  1.00 39.01           B
ATOM   4028  CE2  TYR B 153       5.310  24.696  20.696  1.00 39.82           B
ATOM   4029  CZ   TYR B 153       4.866  25.075  21.915  1.00 40.12           B
ATOM   4030  OH   TYR B 153       5.607  26.030  22.574  1.00 39.51           B
ATOM   4031  C    TYR B 153       4.403  20.171  20.568  1.00 32.24           B
ATOM   4032  O    TYR B 153       4.833  19.616  19.554  1.00 30.69           B
ATOM   4033  N    TYR B 154       5.175  20.445  21.612  1.00 30.25           B
ATOM   4034  CA   TYR B 154       6.585  20.103  21.597  1.00 30.50           B
ATOM   4035  CB   TYR B 154       7.324  20.751  22.779  1.00 32.66           B
ATOM   4036  CG   TYR B 154       6.785  20.471  24.172  1.00 35.85           B
ATOM   4037  CD1  TYR B 154       7.325  19.450  24.953  1.00 36.54           B
ATOM   4038  CE1  TYR B 154       6.888  19.225  26.267  1.00 37.57           B
ATOM   4039  CD2  TYR B 154       5.779  21.270  24.734  1.00 37.28           B
ATOM   4040  CE2  TYR B 154       5.334  21.053  26.047  1.00 37.15           B
ATOM   4041  CZ   TYR B 154       5.895  20.030  26.805  1.00 38.13           B
ATOM   4042  OH   TYR B 154       5.477  19.804  28.098  1.00 38.78           B
ATOM   4043  C    TYR B 154       6.813  18.585  21.571  1.00 29.59           B
ATOM   4044  O    TYR B 154       7.817  18.113  21.040  1.00 28.98           B
ATOM   4045  N    LEU B 155       5.874  17.816  22.109  1.00 27.11           B
ATOM   4046  CA   LEU B 155       6.029  16.359  22.087  1.00 26.11           B
ATOM   4047  CB   LEU B 155       5.055  15.686  23.064  1.00 25.90           B
ATOM   4048  CG   LEU B 155       5.260  16.046  24.536  1.00 27.10           B
ATOM   4049  CD1  LEU B 155       4.256  15.237  25.360  1.00 29.20           B
ATOM   4050  CD2  LEU B 155       6.686  15.757  24.980  1.00 28.73           B
ATOM   4051  C    LEU B 155       5.808  15.776  20.682  1.00 25.64           B
ATOM   4052  O    LEU B 155       6.177  14.613  20.431  1.00 25.89           B
ATOM   4053  N    ASN B 156       5.210  16.560  19.781  1.00 23.01           B
ATOM   4054  CA   ASN B 156       4.962  16.121  18.405  1.00 23.44           B
ATOM   4055  CB   ASN B 156       3.911  16.986  17.737  1.00 25.76           B
ATOM   4056  CG   ASN B 156       2.570  16.900  18.436  1.00 29.20           B
ATOM   4057  OD1  ASN B 156       1.720  17.790  18.296  1.00 30.71           B
ATOM   4058  ND2  ASN B 156       2.373  15.830  19.194  1.00 24.28           B
ATOM   4059  C    ASN B 156       6.235  16.141  17.547  1.00 23.66           B
ATOM   4060  O    ASN B 156       6.203  15.696  16.400  1.00 23.58           B
ATOM   4061  N    GLY B 157       7.332  16.630  18.122  1.00 22.86           B
ATOM   4062  CA   GLY B 157       8.596  16.686  17.399  1.00 22.29           B
ATOM   4063  C    GLY B 157       9.630  15.756  18.000  1.00 22.40           B
ATOM   4064  O    GLY B 157       9.307  14.894  18.819  1.00 21.77           B
ATOM   4065  N    MET B 158      10.890  15.911  17.604  1.00 19.12           B
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Figure 1 (continued 41)

ATOM	4066	CA	MET	B	158	11.963	15.074	18.121	1.00	18.96	B
ATOM	4067	CB	MET	B	158	12.516	14.163	17.003	1.00	16.50	B
ATOM	4068	CG	MET	B	158	13.688	13.297	17.395	1.00	15.32	B
ATOM	4069	SD	MET	B	158	14.254	12.235	16.035	1.00	16.20	B
ATOM	4070	CE	MET	B	158	12.919	10.970	16.029	1.00	15.94	B
ATOM	4071	C	MET	B	158	13.095	15.928	18.658	1.00	19.64	B
ATOM	4072	O	MET	B	158	13.530	16.880	18.006	1.00	18.73	B
ATOM	4073	N	LEU	B	159	13.564	15.621	19.854	1.00	19.03	B
ATOM	4074	CA	LEU	B	159	14.674	16.383	20.397	1.00	19.89	B
ATOM	4075	CB	LEU	B	159	14.747	16.250	21.921	1.00	21.16	B
ATOM	4076	CG	LEU	B	159	15.847	17.145	22.504	1.00	23.17	B
ATOM	4077	CD1	LEU	B	159	15.239	18.525	22.690	1.00	24.44	B
ATOM	4078	CD2	LEU	B	159	16.406	16.575	23.857	1.00	26.60	B
ATOM	4079	C	LEU	B	159	15.999	15.897	19.816	1.00	18.80	B
ATOM	4080	O	LEU	B	159	16.232	14.693	19.707	1.00	19.10	B
ATOM	4081	N	PHE	B	160	16.854	16.844	19.397	1.00	18.54	B
ATOM	4082	CA	PHE	B	160	18.194	16.522	18.906	1.00	18.56	B
ATOM	4083	CB	PHE	B	160	18.414	17.041	17.481	1.00	17.32	B
ATOM	4084	CG	PHE	B	160	17.833	16.158	16.414	1.00	16.68	B
ATOM	4085	CD1	PHE	B	160	16.460	16.129	16.172	1.00	16.33	B
ATOM	4086	CD2	PHE	B	160	18.668	15.338	15.644	1.00	18.29	B
ATOM	4087	CE1	PHE	B	160	15.916	15.291	15.170	1.00	15.09	B
ATOM	4088	CE2	PHE	B	160	18.145	14.498	14.641	1.00	18.37	B
ATOM	4089	CZ	PHE	B	160	16.758	14.474	14.400	1.00	16.02	B
ATOM	4090	C	PHE	B	160	19.169	17.220	19.862	1.00	20.39	B
ATOM	4091	O	PHE	B	160	19.045	18.421	20.088	1.00	22.48	B
ATOM	4092	N	GLU	B	161	20.123	16.472	20.409	1.00	22.11	B
ATOM	4093	CA	GLU	B	161	21.062	17.021	21.371	1.00	23.08	B
ATOM	4094	CB	GLU	B	161	20.595	16.616	22.795	1.00	25.07	B
ATOM	4095	CG	GLU	B	161	21.687	16.649	23.845	1.00	29.45	B
ATOM	4096	CD	GLU	B	161	21.216	16.219	25.237	1.00	32.67	B
ATOM	4097	OE1	GLU	B	161	20.335	15.337	25.350	1.00	33.61	B
ATOM	4098	OE2	GLU	B	161	21.762	16.750	26.232	1.00	35.08	B
ATOM	4099	C	GLU	B	161	22.515	16.620	21.139	1.00	23.37	B
ATOM	4100	O	GLU	B	161	22.817	15.483	20.812	1.00	22.03	B
ATOM	4101	N	THR	B	162	23.422	17.589	21.282	1.00	24.63	B
ATOM	4102	CA	THR	B	162	24.848	17.337	21.145	1.00	26.40	B
ATOM	4103	CB	THR	B	162	25.546	18.444	20.281	1.00	25.08	B
ATOM	4104	OG1	THR	B	162	25.086	19.747	20.676	1.00	24.91	B
ATOM	4105	CG2	THR	B	162	25.223	18.231	18.803	1.00	27.18	B
ATOM	4106	C	THR	B	162	25.438	17.336	22.565	1.00	27.15	B
ATOM	4107	O	THR	B	162	25.127	18.222	23.359	1.00	28.33	B
ATOM	4108	N	GLU	B	163	26.256	16.332	22.881	1.00	29.67	B
ATOM	4109	CA	GLU	B	163	26.883	16.224	24.207	1.00	31.99	B
ATOM	4110	CB	GLU	B	163	25.975	15.463	25.173	1.00	34.55	B
ATOM	4111	CG	GLU	B	163	24.640	16.124	25.426	1.00	37.21	B
ATOM	4112	CD	GLU	B	163	24.739	17.368	26.290	1.00	40.30	B
ATOM	4113	OE1	GLU	B	163	25.272	17.271	27.421	1.00	42.28	B
ATOM	4114	OE2	GLU	B	163	24.272	18.442	25.843	1.00	40.47	B
ATOM	4115	C	GLU	B	163	28.208	15.514	24.119	1.00	31.89	B
ATOM	4116	O	GLU	B	163	28.284	14.360	23.703	1.00	31.49	B
ATOM	4117	N	GLY	B	164	29.263	16.208	24.524	1.00	33.08	B
ATOM	4118	CA	GLY	B	164	30.578	15.612	24.458	1.00	34.03	B
ATOM	4119	C	GLY	B	164	30.958	15.337	23.015	1.00	34.75	B
ATOM	4120	O	GLY	B	164	31.279	16.249	22.251	1.00	35.89	B
ATOM	4121	N	GLU	B	165	30.900	14.070	22.637	1.00	33.48	B
ATOM	4122	CA	GLU	B	165	31.243	13.651	21.296	1.00	33.45	B
ATOM	4123	CB	GLU	B	165	32.465	12.749	21.359	1.00	36.52	B
ATOM	4124	CG	GLU	B	165	32.859	12.136	20.032	1.00	40.64	B
ATOM	4125	CD	GLU	B	165	33.569	10.807	20.209	1.00	41.89	B
ATOM	4126	OE1	GLU	B	165	34.538	10.756	21.003	1.00	45.17	B
ATOM	4127	OE2	GLU	B	165	33.163	9.825	19.552	1.00	42.89	B
ATOM	4128	C	GLU	B	165	30.069	12.886	20.686	1.00	31.49	B
ATOM	4129	O	GLU	B	165	30.216	12.207	19.680	1.00	30.99	B
ATOM	4130	N	GLU	B	166	28.898	12.996	21.301	1.00	31.17	B
ATOM	4131	CA	GLU	B	166	27.734	12.272	20.786	1.00	30.34	B
ATOM	4132	CB	GLU	B	166	27.186	11.327	21.852	1.00	32.23	B
ATOM	4133	CG	GLU	B	166	28.125	10.236	22.339	1.00	35.23	B
ATOM	4134	CD	GLU	B	166	27.417	9.289	23.290	1.00	37.38	B
ATOM	4135	OE1	GLU	B	166	27.041	9.723	24.405	1.00	38.59	B
ATOM	4136	OE2	GLU	B	166	27.218	8.120	22.913	1.00	39.47	B
ATOM	4137	C	GLU	B	166	26.570	13.156	20.329	1.00	27.86	B
ATOM	4138	O	GLU	B	166	26.408	14.273	20.797	1.00	27.41	B
ATOM	4139	N	LEU	B	167	25.776	12.628	19.397	1.00	25.92	B
ATOM	4140	CA	LEU	B	167	24.560	13.291	18.930	1.00	23.86	B
ATOM	4141	CB	LEU	B	167	24.455	13.313	17.402	1.00	23.73	B
ATOM	4142	CG	LEU	B	167	23.631	14.415	16.685	1.00	24.90	B
ATOM	4143	CD1	LEU	B	167	23.059	13.834	15.415	1.00	21.07	B
ATOM	4144	CD2	LEU	B	167	22.555	15.041	17.534	1.00	23.85	B
ATOM	4145	C	LEU	B	167	23.520	12.303	19.481	1.00	21.77	B
ATOM	4146	O	LEU	B	167	23.705	11.083	19.405	1.00	22.32	B
ATOM	4147	N	ARG	B	168	22.439	12.834	20.021	1.00	21.49	B
ATOM	4148	CA	ARG	B	168	21.393	11.996	20.596	1.00	21.70	B
ATOM	4149	CB	ARG	B	168	21.549	12.047	22.117	1.00	24.79	B
ATOM	4150	CG	ARG	B	168	20.309	11.678	22.928	1.00	27.63	B
ATOM	4151	CD	ARG	B	168	20.635	11.575	24.419	1.00	31.15	B
ATOM	4152	NE	ARG	B	168	21.104	12.813	25.018	1.00	33.80	B
ATOM	4153	CZ	ARG	B	168	22.333	13.005	25.502	1.00	33.14	B
ATOM	4154	NH1	ARG	B	168	23.245	12.040	25.466	1.00	33.70	B
ATOM	4155	NH2	ARG	B	168	22.646	14.169	26.022	1.00	34.73	B
ATOM	4156	C	ARG	B	168	20.001	12.475	20.188	1.00	20.94	B
ATOM	4157	O	ARG	B	168	19.782	13.664	19.977	1.00	20.05	B
ATOM	4158	N	THR	B	169	19.059	11.549	20.026	1.00	18.53	B
ATOM	4159	CA	THR	B	169	17.693	11.945	19.748	1.00	17.19	B
ATOM	4160	CB	THR	B	169	17.141	11.377	18.420	1.00	17.29	B
ATOM	4161	OG1	THR	B	169	17.290	9.961	18.415	1.00	17.62	B
ATOM	4162	CG2	THR	B	169	17.936	11.920	17.241	1.00	17.89	B
ATOM	4163	C	THR	B	169	16.846	11.382	20.870	1.00	18.82	B
ATOM	4164	O	THR	B	169	17.200	10.356	21.474	1.00	18.41	B
ATOM	4165	N	VAL	B	170	15.772	12.095	21.151	1.00	18.62	B

Figure 1 (continued 42)

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ATOM   4166   CA    VAL B 170      14.796   11.705   22.176   1.00  18.28        B
ATOM   4167   CB    VAL B 170      15.031   12.497   23.489   1.00  17.76        B
ATOM   4168   CG1   VAL B 170      14.085   11.948   24.589   1.00  18.88        B
ATOM   4169   CG2   VAL B 170      16.520   12.397   23.913   1.00  18.42        B
ATOM   4170   C     VAL B 170      13.368   11.981   21.674   1.00  18.46        B
ATOM   4171   O     VAL B 170      13.087   13.010   21.060   1.00  18.89        B
ATOM   4172   N     ALA B 171      12.455   11.031   21.908   1.00  15.83        B
ATOM   4173   CA    ALA B 171      11.069   11.206   21.518   1.00  16.19        B
ATOM   4174   CB    ALA B 171      10.771   10.503   20.212   1.00  16.47        B
ATOM   4175   C     ALA B 171      10.234   10.606   22.617   1.00  17.41        B
ATOM   4176   O     ALA B 171      10.642    9.616   23.213   1.00  18.10        B
ATOM   4177   N     THR B 172       9.112   11.246   22.902   1.00  16.52        B
ATOM   4178   CA    THR B 172       8.212   10.730   23.917   1.00  17.52        B
ATOM   4179   CB    THR B 172       8.776   11.014   25.344   1.00  18.95        B
ATOM   4180   OG1   THR B 172       7.931   10.400   26.328   1.00  19.33        B
ATOM   4181   CG2   THR B 172       8.870   12.532   25.619   1.00  18.29        B
ATOM   4182   C     THR B 172       6.805   11.269   23.709   1.00  18.84        B
ATOM   4183   O     THR B 172       6.588   12.352   23.145   1.00  20.21        B
ATOM   4184   N     ASP B 173       5.820   10.481   24.134   1.00  18.12        B
ATOM   4185   CA    ASP B 173       4.447   10.902   23.972   1.00  19.17        B
ATOM   4186   CB    ASP B 173       3.709    9.980   22.996   1.00  19.41        B
ATOM   4187   CG    ASP B 173       3.663    8.531   23.461   1.00  19.37        B
ATOM   4188   OD1   ASP B 173       4.197    8.212   24.540   1.00  20.26        B
ATOM   4189   OD2   ASP B 173       3.087    7.712   22.710   1.00  18.53        B
ATOM   4190   C     ASP B 173       3.766   10.895   25.336   1.00  19.52        B
ATOM   4191   O     ASP B 173       2.546   11.011   25.408   1.00  22.03        B
ATOM   4192   N     GLY B 174       4.562   10.770   26.397   1.00  20.37        B
ATOM   4193   CA    GLY B 174       3.992   10.745   27.737   1.00  22.96        B
ATOM   4194   C     GLY B 174       3.762    9.337   28.266   1.00  24.51        B
ATOM   4195   O     GLY B 174       3.667    9.141   29.489   1.00  26.84        B
ATOM   4196   N     HIS B 175       3.650    8.349   27.375   1.00  23.92        B
ATOM   4197   CA    HIS B 175       3.440    6.953   27.796   1.00  22.95        B
ATOM   4198   CB    HIS B 175       2.313    6.309   26.977   1.00  25.89        B
ATOM   4199   CG    HIS B 175       0.992    6.997   27.119   1.00  28.87        B
ATOM   4200   CD2   HIS B 175       0.106    7.435   26.193   1.00  30.90        B
ATOM   4201   ND1   HIS B 175       0.420    7.255   28.345   1.00  30.54        B
ATOM   4202   CE1   HIS B 175      -0.763    7.817   28.170   1.00  28.94        B
ATOM   4203   NE2   HIS B 175      -0.977    7.938   26.875   1.00  31.49        B
ATOM   4204   C     HIS B 175       4.706    6.135   27.641   1.00  23.03        B
ATOM   4205   O     HIS B 175       4.990    5.212   28.403   1.00  22.08        B
ATOM   4206   N     ARG B 176       5.481    6.461   26.617   1.00  18.76        B
ATOM   4207   CA    ARG B 176       6.711    5.768   26.422   1.00  18.30        B
ATOM   4208   CB    ARG B 176       6.575    4.633   25.398   1.00  19.53        B
ATOM   4209   CG    ARG B 176       6.329    5.094   23.954   1.00  22.88        B
ATOM   4210   CD    ARG B 176       4.876    4.888   23.657   1.00  22.11        B
ATOM   4211   NE    ARG B 176       4.435    5.312   22.314   1.00  22.09        B
ATOM   4212   CZ    ARG B 176       4.555    4.591   21.202   1.00  20.17        B
ATOM   4213   NH1   ARG B 176       5.159    3.403   21.213   1.00  17.04        B
ATOM   4214   NH2   ARG B 176       3.914    4.977   20.120   1.00  20.02        B
ATOM   4215   C     ARG B 176       7.684    6.807   25.902   1.00  17.30        B
ATOM   4216   O     ARG B 176       7.255    7.860   25.374   1.00  18.10        B
ATOM   4217   N     LEU B 177       8.957    6.504   26.080   1.00  17.97        B
ATOM   4218   CA    LEU B 177      10.049    7.360   25.633   1.00  17.85        B
ATOM   4219   CB    LEU B 177      10.664    8.095   26.827   1.00  18.29        B
ATOM   4220   CG    LEU B 177      11.921    8.955   26.611   1.00  16.28        B
ATOM   4221   CD1   LEU B 177      11.819   10.163   27.559   1.00  19.52        B
ATOM   4222   CD2   LEU B 177      13.191    8.172   26.839   1.00  19.12        B
ATOM   4223   C     LEU B 177      11.110    6.517   24.964   1.00  18.45        B
ATOM   4224   O     LEU B 177      11.291    5.329   25.281   1.00  18.33        B
ATOM   4225   N     ALA B 178      11.801    7.131   24.006   1.00  15.84        B
ATOM   4226   CA    ALA B 178      12.899    6.489   23.308   1.00  15.12        B
ATOM   4227   CB    ALA B 178      12.495    6.133   21.883   1.00  13.82        B
ATOM   4228   C     ALA B 178      14.041    7.488   23.279   1.00  15.48        B
ATOM   4229   O     ALA B 178      13.797    8.670   23.063   1.00  17.09        B
ATOM   4230   N     VAL B 179      15.258    7.014   23.546   1.00  17.40        B
ATOM   4231   CA    VAL B 179      16.470    7.851   23.508   1.00  18.38        B
ATOM   4232   CB    VAL B 179      16.881    8.318   24.937   1.00  18.67        B
ATOM   4233   CG1   VAL B 179      17.294    7.120   25.770   1.00  19.18        B
ATOM   4234   CG2   VAL B 179      18.060    9.286   24.864   1.00  20.37        B
ATOM   4235   C     VAL B 179      17.590    7.037   22.849   1.00  19.44        B
ATOM   4236   O     VAL B 179      17.737    5.829   23.092   1.00  19.37        B
ATOM   4237   N     CYS B 180      18.370    7.676   21.968   1.00  17.08        B
ATOM   4238   CA    CYS B 180      19.434    6.979   21.293   1.00  18.58        B
ATOM   4239   CB    CYS B 180      18.961    6.489   19.918   1.00  17.06        B
ATOM   4240   SG    CYS B 180      20.198    5.643   18.973   1.00  22.31        B
ATOM   4241   C     CYS B 180      20.602    7.948   21.135   1.00  19.35        B
ATOM   4242   O     CYS B 180      20.405    9.093   20.736   1.00  19.68        B
ATOM   4243   N     SER B 181      21.798    7.464   21.442   1.00  21.74        B
ATOM   4244   CA    SER B 181      23.015    8.277   21.369   1.00  25.46        B
ATOM   4245   CB    SER B 181      23.615    8.457   22.774   1.00  28.11        B
ATOM   4246   OG    SER B 181      22.674    9.033   23.654   1.00  30.74        B
ATOM   4247   C     SER B 181      24.037    7.590   20.498   1.00  26.06        B
ATOM   4248   O     SER B 181      24.182    6.370   20.554   1.00  25.12        B
ATOM   4249   N     MET B 182      24.765    8.374   19.704   1.00  25.90        B
ATOM   4250   CA    MET B 182      25.779    7.846   18.813   1.00  29.20        B
ATOM   4251   CB    MET B 182      25.238    7.784   17.382   1.00  31.43        B
ATOM   4252   CG    MET B 182      24.114    6.789   17.181   1.00  33.69        B
ATOM   4253   SD    MET B 182      24.722    5.139   17.524   1.00  34.88        B
ATOM   4254   CE    MET B 182      25.373    4.651   15.929   1.00  34.59        B
ATOM   4255   C     MET B 182      27.001    8.758   18.834   1.00  30.52        B
ATOM   4256   O     MET B 182      26.857    9.983   18.819   1.00  30.18        B
ATOM   4257   N     PRO B 183      28.214    8.177   18.872   1.00  32.39        B
ATOM   4258   CD    PRO B 183      28.529    6.737   18.860   1.00  34.00        B
ATOM   4259   CA    PRO B 183      29.449    8.977   18.888   1.00  34.40        B
ATOM   4260   CB    PRO B 183      30.521    7.940   19.199   1.00  34.66        B
ATOM   4261   CG    PRO B 183      29.998    6.735   18.481   1.00  35.09        B
ATOM   4262   C     PRO B 183      29.663    9.624   17.517   1.00  35.33        B
ATOM   4263   O     PRO B 183      29.355    9.015   16.502   1.00  35.46        B
ATOM   4264   N     ILE B 184      30.199   10.843   17.506   1.00  36.88        B
ATOM   4265   CA    ILE B 184      30.445   11.589   16.271   1.00  38.38        B
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Figure 1 (continued 43)

ATOM	4266	CB	ILE	B	184	29.676	12.942	16.305	1.00	37.59	B
ATOM	4267	CG2	ILE	B	184	30.131	13.872	15.192	1.00	39.18	B
ATOM	4268	CG1	ILE	B	184	28.185	12.670	16.154	1.00	39.46	B
ATOM	4269	CD1	ILE	B	184	27.857	11.818	14.939	1.00	38.79	B
ATOM	4270	C	ILE	B	184	31.926	11.864	15.976	1.00	39.26	B
ATOM	4271	O	ILE	B	184	32.266	12.371	14.913	1.00	39.33	B
ATOM	4272	N	GLY	B	185	32.810	11.528	16.906	1.00	40.53	B
ATOM	4273	CA	GLY	B	185	34.225	11.777	16.671	1.00	42.10	B
ATOM	4274	C	GLY	B	185	34.630	13.227	16.897	1.00	43.16	B
ATOM	4275	O	GLY	B	185	35.821	13.542	16.982	1.00	44.33	B
ATOM	4276	N	GLN	B	186	33.646	14.117	16.988	1.00	43.84	B
ATOM	4277	CA	GLN	B	186	33.898	15.541	17.208	1.00	44.08	B
ATOM	4278	CB	GLN	B	186	33.069	16.406	16.254	1.00	43.89	B
ATOM	4279	CG	GLN	B	186	33.456	16.388	14.800	1.00	44.39	B
ATOM	4280	CD	GLN	B	186	32.677	17.426	14.006	1.00	43.95	B
ATOM	4281	OE1	GLN	B	186	32.773	18.631	14.269	1.00	44.45	B
ATOM	4282	NE2	GLN	B	186	31.893	16.963	13.039	1.00	42.44	B
ATOM	4283	C	GLN	B	186	33.503	15.952	18.614	1.00	44.05	B
ATOM	4284	O	GLN	B	186	32.650	15.325	19.228	1.00	44.15	B
ATOM	4285	N	SER	B	187	34.115	17.019	19.115	1.00	43.83	B
ATOM	4286	CA	SER	B	187	33.779	17.544	20.434	1.00	43.99	B
ATOM	4287	CB	SER	B	187	35.025	18.105	21.138	1.00	44.53	B
ATOM	4288	OG	SER	B	187	36.033	17.117	21.304	1.00	45.53	B
ATOM	4289	C	SER	B	187	32.797	18.675	20.121	1.00	43.54	B
ATOM	4290	O	SER	B	187	33.117	19.573	19.338	1.00	43.42	B
ATOM	4291	N	LEU	B	188	31.603	18.635	20.705	1.00	42.54	B
ATOM	4292	CA	LEU	B	188	30.616	19.669	20.425	1.00	41.93	B
ATOM	4293	CB	LEU	B	188	29.425	19.083	19.652	1.00	42.36	B
ATOM	4294	CG	LEU	B	188	29.558	18.823	18.148	1.00	42.40	B
ATOM	4295	CD1	LEU	B	188	30.321	19.973	17.494	1.00	42.81	B
ATOM	4296	CD2	LEU	B	188	30.269	17.515	17.910	1.00	42.43	B
ATOM	4297	C	LEU	B	188	30.074	20.411	21.623	1.00	41.46	B
ATOM	4298	O	LEU	B	188	30.097	19.910	22.742	1.00	42.28	B
ATOM	4299	N	PRO	B	189	29.580	21.638	21.398	1.00	40.92	B
ATOM	4300	CD	PRO	B	189	29.691	22.410	20.147	1.00	40.91	B
ATOM	4301	CA	PRO	B	189	29.009	22.457	22.466	1.00	39.91	B
ATOM	4302	CB	PRO	B	189	28.784	23.810	21.793	1.00	40.82	B
ATOM	4303	CG	PRO	B	189	29.770	23.819	20.656	1.00	41.55	B
ATOM	4304	C	PRO	B	189	27.683	21.801	22.853	1.00	39.55	B
ATOM	4305	O	PRO	B	189	26.834	21.544	21.995	1.00	37.81	B
ATOM	4306	N	SER	B	190	27.507	21.512	24.134	1.00	38.79	B
ATOM	4307	CA	SER	B	190	26.266	20.889	24.577	1.00	38.03	B
ATOM	4308	CB	SER	B	190	26.237	20.860	26.103	1.00	38.64	B
ATOM	4309	OG	SER	B	190	27.459	20.337	26.593	1.00	41.63	B
ATOM	4310	C	SER	B	190	25.126	21.733	24.005	1.00	36.48	B
ATOM	4311	O	SER	B	190	25.072	22.937	24.221	1.00	37.47	B
ATOM	4312	N	HIS	B	191	24.214	21.102	23.268	1.00	34.74	B
ATOM	4313	CA	HIS	B	191	23.122	21.831	22.620	1.00	32.42	B
ATOM	4314	CB	HIS	B	191	23.568	22.172	21.214	1.00	33.72	B
ATOM	4315	CG	HIS	B	191	23.168	23.535	20.772	1.00	34.73	B
ATOM	4316	CD2	HIS	B	191	22.084	23.968	20.094	1.00	35.24	B
ATOM	4317	ND1	HIS	B	191	23.936	24.649	21.031	1.00	35.16	B
ATOM	4318	CE1	HIS	B	191	23.339	25.714	20.527	1.00	36.06	B
ATOM	4319	NE2	HIS	B	191	22.212	25.328	19.955	1.00	35.42	B
ATOM	4320	C	HIS	B	191	21.803	21.029	22.537	1.00	31.03	B
ATOM	4321	O	HIS	B	191	21.851	19.831	22.375	1.00	31.38	B
ATOM	4322	N	SER	B	192	20.649	21.695	22.605	1.00	29.69	B
ATOM	4323	CA	SER	B	192	19.354	20.993	22.547	1.00	28.86	B
ATOM	4324	CB	SER	B	192	18.819	20.691	23.955	1.00	28.56	B
ATOM	4325	OG	SER	B	192	19.649	19.762	24.617	1.00	32.04	B
ATOM	4326	C	SER	B	192	18.239	21.687	21.801	1.00	28.26	B
ATOM	4327	O	SER	B	192	17.764	22.768	22.223	1.00	29.68	B
ATOM	4328	N	VAL	B	193	17.765	21.042	20.731	1.00	23.60	B
ATOM	4329	CA	VAL	B	193	16.676	21.602	19.942	1.00	22.38	B
ATOM	4330	CB	VAL	B	193	17.198	22.242	18.651	1.00	20.07	B
ATOM	4331	CG1	VAL	B	193	18.139	23.408	18.996	1.00	22.51	B
ATOM	4332	CG2	VAL	B	193	17.914	21.209	17.824	1.00	21.46	B
ATOM	4333	C	VAL	B	193	15.618	20.598	19.542	1.00	21.51	B
ATOM	4334	O	VAL	B	193	15.877	19.389	19.444	1.00	20.75	B
ATOM	4335	N	ILE	B	194	14.431	21.113	19.297	1.00	19.19	B
ATOM	4336	CA	ILE	B	194	13.300	20.279	18.885	1.00	18.69	B
ATOM	4337	CB	ILE	B	194	12.047	20.662	19.661	1.00	20.65	B
ATOM	4338	CG2	ILE	B	194	10.879	19.737	19.263	1.00	20.91	B
ATOM	4339	CG1	ILE	B	194	12.351	20.584	21.156	1.00	22.06	B
ATOM	4340	CD1	ILE	B	194	11.268	21.174	21.991	1.00	25.62	B
ATOM	4341	C	ILE	B	194	13.025	20.452	17.392	1.00	17.66	B
ATOM	4342	O	ILE	B	194	12.699	21.535	16.925	1.00	17.42	B
ATOM	4343	N	VAL	B	195	13.147	19.361	16.641	1.00	17.07	B
ATOM	4344	CA	VAL	B	195	12.878	19.360	15.212	1.00	15.23	B
ATOM	4345	CB	VAL	B	195	13.834	18.401	14.473	1.00	17.30	B
ATOM	4346	CG1	VAL	B	195	13.491	18.338	12.979	1.00	16.64	B
ATOM	4347	CG2	VAL	B	195	15.268	18.857	14.695	1.00	16.68	B
ATOM	4348	C	VAL	B	195	11.412	18.916	15.005	1.00	16.31	B
ATOM	4349	O	VAL	B	195	10.978	17.903	15.567	1.00	16.90	B
ATOM	4350	N	PRO	B	196	10.632	19.670	14.207	1.00	17.47	B
ATOM	4351	CD	PRO	B	196	11.074	20.815	13.395	1.00	18.83	B
ATOM	4352	CA	PRO	B	196	9.215	19.364	13.933	1.00	19.05	B
ATOM	4353	CB	PRO	B	196	8.772	20.478	12.980	1.00	20.57	B
ATOM	4354	CG	PRO	B	196	9.793	21.504	13.114	1.00	22.10	B
ATOM	4355	C	PRO	B	196	9.046	18.009	13.265	1.00	19.72	B
ATOM	4356	O	PRO	B	196	9.944	17.513	12.607	1.00	18.66	B
ATOM	4357	N	ARG	B	197	7.862	17.440	13.430	1.00	20.21	B
ATOM	4358	CA	ARG	B	197	7.519	16.149	12.846	1.00	21.19	B
ATOM	4359	CB	ARG	B	197	6.012	15.904	13.000	1.00	25.71	B
ATOM	4360	CG	ARG	B	197	5.519	14.646	12.322	1.00	30.00	B
ATOM	4361	CD	ARG	B	197	3.984	14.652	12.252	1.00	32.19	B
ATOM	4362	NE	ARG	B	197	3.458	15.525	11.200	1.00	35.51	B
ATOM	4363	CZ	ARG	B	197	3.290	15.155	9.929	1.00	36.04	B
ATOM	4364	NH1	ARG	B	197	3.606	13.925	9.536	1.00	36.85	B
ATOM	4365	NH2	ARG	B	197	2.793	16.012	9.051	1.00	37.72	B

Figure 1 (continued 44)

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ATOM   4366  C   ARG B 197      7.873  16.032  11.374  1.00 20.20      B
ATOM   4367  O   ARG B 197      8.529  15.075  10.978  1.00 18.75      B
ATOM   4368  N   LYS B 198      7.426  16.982  10.553  1.00 19.22      B
ATOM   4369  CA  LYS B 198      7.713  16.900   9.122  1.00 20.05      B
ATOM   4370  CB  LYS B 198      6.956  17.965   8.323  1.00 22.68      B
ATOM   4371  CG  LYS B 198      5.458  17.685   8.160  1.00 27.88      B
ATOM   4372  CD  LYS B 198      4.815  18.821   7.335  1.00 32.73      B
ATOM   4373  CE  LYS B 198      3.313  18.648   7.098  1.00 36.66      B
ATOM   4374  NZ  LYS B 198      2.468  18.767   8.340  1.00 38.58      B
ATOM   4375  C   LYS B 198      9.190  17.058   8.872  1.00 17.68      B
ATOM   4376  O   LYS B 198      9.709  16.583   7.873  1.00 19.10      B
ATOM   4377  N   GLY B 199      9.866  17.731   9.790  1.00 15.43      B
ATOM   4378  CA  GLY B 199     11.292  17.946   9.628  1.00 16.07      B
ATOM   4379  C   GLY B 199     12.045  16.641   9.766  1.00 15.66      B
ATOM   4380  O   GLY B 199     13.015  16.380   9.059  1.00 15.20      B
ATOM   4381  N   VAL B 200     11.624  15.841  10.737  1.00 14.98      B
ATOM   4382  CA  VAL B 200     12.245  14.548  10.958  1.00 15.69      B
ATOM   4383  CB  VAL B 200     11.617  13.864  12.175  1.00 16.41      B
ATOM   4384  CG1 VAL B 200     12.217  12.449  12.354  1.00 18.05      B
ATOM   4385  CG2 VAL B 200     11.899  14.718  13.380  1.00 17.11      B
ATOM   4386  C   VAL B 200     12.056  13.678   9.722  1.00 15.55      B
ATOM   4387  O   VAL B 200     12.977  12.967   9.284  1.00 17.07      B
ATOM   4388  N   ILE B 201     10.858  13.703   9.165  1.00 18.07      B
ATOM   4389  CA  ILE B 201     10.567  12.942   7.950  1.00 18.45      B
ATOM   4390  CB  ILE B 201      9.084  13.098   7.563  1.00 19.51      B
ATOM   4391  CG2 ILE B 201      8.814  12.494   6.175  1.00 21.46      B
ATOM   4392  CG1 ILE B 201      8.238  12.391   8.602  1.00 20.58      B
ATOM   4393  CD1 ILE B 201      6.738  12.554   8.392  1.00 24.22      B
ATOM   4394  C   ILE B 201     11.447  13.367   6.789  1.00 18.72      B
ATOM   4395  O   ILE B 201     11.960  12.519   6.065  1.00 20.22      B
ATOM   4396  N   GLU B 202     11.643  14.673   6.607  1.00 19.15      B
ATOM   4397  CA  GLU B 202     12.483  15.152   5.514  1.00 20.05      B
ATOM   4398  CB  GLU B 202     12.426  16.681   5.362  1.00 21.56      B
ATOM   4399  CG  GLU B 202     11.174  17.168   4.689  1.00 24.74      B
ATOM   4400  CD  GLU B 202     10.866  16.349   3.452  1.00 27.41      B
ATOM   4401  OE1 GLU B 202      9.725  15.850   3.346  1.00 27.85      B
ATOM   4402  OE2 GLU B 202     11.770  16.185   2.602  1.00 28.02      B
ATOM   4403  C   GLU B 202     13.923  14.751   5.734  1.00 20.02      B
ATOM   4404  O   GLU B 202     14.602  14.397   4.773  1.00 21.05      B
ATOM   4405  N   LEU B 203     14.405  14.838   6.979  1.00 18.48      B
ATOM   4406  CA  LEU B 203     15.780  14.445   7.272  1.00 19.51      B
ATOM   4407  CB  LEU B 203     16.102  14.570   8.764  1.00 20.96      B
ATOM   4408  CG  LEU B 203     16.378  15.983   9.271  1.00 22.79      B
ATOM   4409  CD1 LEU B 203     16.571  15.960  10.797  1.00 23.58      B
ATOM   4410  CD2 LEU B 203     17.644  16.526   8.566  1.00 24.88      B
ATOM   4411  C   LEU B 203     15.987  13.009   6.848  1.00 20.44      B
ATOM   4412  O   LEU B 203     17.008  12.674   6.231  1.00 18.72      B
ATOM   4413  N   MET B 204     15.027  12.142   7.171  1.00 18.16      B
ATOM   4414  CA  MET B 204     15.153  10.734   6.784  1.00 21.15      B
ATOM   4415  CB  MET B 204     14.008   9.914   7.399  1.00 23.53      B
ATOM   4416  CG  MET B 204     13.959   8.461   6.938  1.00 29.56      B
ATOM   4417  SD  MET B 204     15.384   7.475   7.480  1.00 38.65      B
ATOM   4418  CE  MET B 204     15.782   8.308   8.992  1.00 30.14      B
ATOM   4419  C   MET B 204     15.147  10.530   5.265  1.00 22.14      B
ATOM   4420  O   MET B 204     15.920   9.728   4.732  1.00 22.11      B
ATOM   4421  N   ARG B 205     14.278  11.264   4.579  1.00 22.90      B
ATOM   4422  CA  ARG B 205     14.147  11.174   3.132  1.00 25.90      B
ATOM   4423  CB  ARG B 205     13.008  12.052   2.631  1.00 28.24      B
ATOM   4424  CG  ARG B 205     11.659  11.451   2.747  1.00 31.40      B
ATOM   4425  CD  ARG B 205     10.612  12.462   2.312  1.00 33.52      B
ATOM   4426  NE  ARG B 205      9.282  11.913   2.527  1.00 34.98      B
ATOM   4427  CZ  ARG B 205      8.155  12.614   2.484  1.00 36.39      B
ATOM   4428  NH1 ARG B 205      8.186  13.912   2.228  1.00 36.54      B
ATOM   4429  NH2 ARG B 205      6.997  12.008   2.717  1.00 36.70      B
ATOM   4430  C   ARG B 205     15.360  11.583   2.355  1.00 26.12      B
ATOM   4431  O   ARG B 205     15.548  11.131   1.226  1.00 25.57      B
ATOM   4432  N   MET B 206     16.182  12.453   2.923  1.00 25.37      B
ATOM   4433  CA  MET B 206     17.332  12.907   2.167  1.00 26.52      B
ATOM   4434  CB  MET B 206     17.690  14.334   2.563  1.00 27.58      B
ATOM   4435  CG  MET B 206     18.358  14.497   3.881  1.00 25.49      B
ATOM   4436  SD  MET B 206     18.341  16.237   4.294  1.00 27.01      B
ATOM   4437  CE  MET B 206     18.905  16.967   2.700  1.00 25.57      B
ATOM   4438  C   MET B 206     18.541  12.008   2.269  1.00 27.45      B
ATOM   4439  O   MET B 206     19.584  12.282   1.669  1.00 26.91      B
ATOM   4440  N   LEU B 207     18.407  10.934   3.036  1.00 28.07      B
ATOM   4441  CA  LEU B 207     19.512  10.010   3.172  1.00 30.58      B
ATOM   4442  CB  LEU B 207     19.407   9.290   4.512  1.00 29.11      B
ATOM   4443  CG  LEU B 207     19.312  10.219   5.724  1.00 26.96      B
ATOM   4444  CD1 LEU B 207     19.271   9.343   6.995  1.00 27.09      B
ATOM   4445  CD2 LEU B 207     20.482  11.190   5.763  1.00 24.96      B
ATOM   4446  C   LEU B 207     19.442   9.029   2.000  1.00 33.44      B
ATOM   4447  O   LEU B 207     18.468   8.306   1.835  1.00 34.23      B
ATOM   4448  N   ASP B 208     20.476   9.020   1.170  1.00 37.29      B
ATOM   4449  CA  ASP B 208     20.490   8.136   0.016  1.00 40.97      B
ATOM   4450  CB  ASP B 208     21.349   8.726  -1.099  1.00 42.41      B
ATOM   4451  CG  ASP B 208     22.832   8.627  -0.799  1.00 43.64      B
ATOM   4452  OD1 ASP B 208     23.355   9.451  -0.024  1.00 45.03      B
ATOM   4453  OD2 ASP B 208     23.483   7.705  -1.330  1.00 46.54      B
ATOM   4454  C   ASP B 208     21.079   6.806   0.437  1.00 42.45      B
ATOM   4455  O   ASP B 208     20.948   5.805  -0.266  1.00 44.07      B
ATOM   4456  N   GLY B 209     21.728   6.795   1.593  1.00 43.63      B
ATOM   4457  CA  GLY B 209     22.347   5.573   2.055  1.00 45.09      B
ATOM   4458  C   GLY B 209     23.590   5.341   1.220  1.00 45.45      B
ATOM   4459  O   GLY B 209     23.921   4.207   0.865  1.00 46.37      B
ATOM   4460  N   GLY B 210     24.273   6.434   0.892  1.00 45.49      B
ATOM   4461  CA  GLY B 210     25.489   6.350   0.111  1.00 44.86      B
ATOM   4462  C   GLY B 210     26.648   6.835   0.952  1.00 44.61      B
ATOM   4463  O   GLY B 210     26.506   7.031   2.158  1.00 44.29      B
ATOM   4464  N   ASP B 211     27.793   7.036   0.311  1.00 44.84      B
ATOM   4465  CA  ASP B 211     28.998   7.499   0.985  1.00 44.68      B
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Figure 1 (continued 45)

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ATOM   4466  CB   ASP B 211      30.220    7.108    0.154   1.00 46.96        B
ATOM   4467  CG   ASP B 211      30.015    7.377   -1.327   1.00 49.59        B
ATOM   4468  OD1  ASP B 211      29.929    8.565   -1.718   1.00 51.33        B
ATOM   4469  OD2  ASP B 211      29.924    6.398   -2.100   1.00 51.23        B
ATOM   4470  C    ASP B 211      29.023    9.008    1.253   1.00 43.00        B
ATOM   4471  O    ASP B 211      29.901    9.493    1.970   1.00 42.86        B
ATOM   4472  N    ASN B 212      28.082    9.758    0.679   1.00 40.95        B
ATOM   4473  CA   ASN B 212      28.054   11.201    0.917   1.00 38.13        B
ATOM   4474  CB   ASN B 212      26.875   11.872    0.200   1.00 40.65        B
ATOM   4475  CG   ASN B 212      26.909   11.679   -1.298   1.00 42.99        B
ATOM   4476  OD1  ASN B 212      26.795   10.553   -1.799   1.00 46.74        B
ATOM   4477  ND2  ASN B 212      27.064   12.774   -2.026   1.00 43.95        B
ATOM   4478  C    ASN B 212      27.891   11.442    2.417   1.00 35.10        B
ATOM   4479  O    ASN B 212      27.031   10.845    3.062   1.00 34.26        B
ATOM   4480  N    PRO B 213      28.722   12.313    2.992   1.00 32.02        B
ATOM   4481  CD   PRO B 213      29.862   13.029    2.379   1.00 33.01        B
ATOM   4482  CA   PRO B 213      28.622   12.604    4.422   1.00 29.13        B
ATOM   4483  CB   PRO B 213      29.993   13.183    4.742   1.00 31.02        B
ATOM   4484  CG   PRO B 213      30.301   13.958    3.492   1.00 31.64        B
ATOM   4485  C    PRO B 213      27.493   13.627    4.641   1.00 26.76        B
ATOM   4486  O    PRO B 213      27.099   14.330    3.711   1.00 25.59        B
ATOM   4487  N    LEU B 214      26.964   13.676    5.856   1.00 23.19        B
ATOM   4488  CA   LEU B 214      25.892   14.608    6.189   1.00 22.69        B
ATOM   4489  CB   LEU B 214      24.805   13.875    7.006   1.00 25.15        B
ATOM   4490  CG   LEU B 214      23.706   14.726    7.624   1.00 27.21        B
ATOM   4491  CD1  LEU B 214      22.868   15.298    6.520   1.00 28.20        B
ATOM   4492  CD2  LEU B 214      22.840   13.877    8.557   1.00 27.67        B
ATOM   4493  C    LEU B 214      26.465   15.766    6.993   1.00 21.63        B
ATOM   4494  O    LEU B 214      27.109   15.551    8.008   1.00 22.98        B
ATOM   4495  N    ARG B 215      26.255   17.004    6.540   1.00 20.26        B
ATOM   4496  CA   ARG B 215      26.763   18.148    7.275   1.00 20.31        B
ATOM   4497  CB   ARG B 215      27.529   19.121    6.367   1.00 24.44        B
ATOM   4498  CG   ARG B 215      28.163   20.269    7.151   1.00 28.96        B
ATOM   4499  CD   ARG B 215      29.021   21.199    6.288   1.00 34.52        B
ATOM   4500  NE   ARG B 215      28.826   22.593    6.691   1.00 38.13        B
ATOM   4501  CZ   ARG B 215      28.386   23.555    5.879   1.00 39.89        B
ATOM   4502  NH1  ARG B 215      28.100   23.297    4.605   1.00 41.19        B
ATOM   4503  NH2  ARG B 215      28.197   24.775    6.352   1.00 42.36        B
ATOM   4504  C    ARG B 215      25.607   18.863    7.923   1.00 19.25        B
ATOM   4505  O    ARG B 215      24.672   19.274    7.253   1.00 19.32        B
ATOM   4506  N    VAL B 216      25.702   19.027    9.231   1.00 16.59        B
ATOM   4507  CA   VAL B 216      24.645   19.655   10.002   1.00 16.36        B
ATOM   4508  CB   VAL B 216      24.224   18.737   11.177   1.00 15.73        B
ATOM   4509  CG1  VAL B 216      23.045   19.383   11.949   1.00 16.54        B
ATOM   4510  CG2  VAL B 216      23.924   17.379   10.674   1.00 16.55        B
ATOM   4511  C    VAL B 216      25.029   20.994   10.583   1.00 18.40        B
ATOM   4512  O    VAL B 216      26.137   21.168   11.094   1.00 18.97        B
ATOM   4513  N    GLN B 217      24.104   21.951   10.521   1.00 16.54        B
ATOM   4514  CA   GLN B 217      24.331   23.265   11.096   1.00 18.52        B
ATOM   4515  CB   GLN B 217      24.482   24.346   10.021   1.00 19.71        B
ATOM   4516  CG   GLN B 217      25.754   24.294    9.206   1.00 21.74        B
ATOM   4517  CD   GLN B 217      25.778   25.415    8.168   1.00 24.98        B
ATOM   4518  OB1  GLN B 217      26.529   26.403    8.299   1.00 28.72        B
ATOM   4519  NE2  GLN B 217      24.932   25.283    7.141   1.00 23.49        B
ATOM   4520  C    GLN B 217      23.088   23.566   11.929   1.00 18.28        B
ATOM   4521  O    GLN B 217      21.970   23.360   11.466   1.00 17.82        B
ATOM   4522  N    ILE B 218      23.293   23.999   13.170   1.00 17.89        B
ATOM   4523  CA   ILE B 218      22.184   24.327   14.049   1.00 18.52        B
ATOM   4524  CB   ILE B 218      22.125   23.382   15.290   1.00 19.36        B
ATOM   4525  CG2  ILE B 218      20.877   23.687   16.133   1.00 21.63        B
ATOM   4526  CG1  ILE B 218      22.098   21.932   14.849   1.00 19.91        B
ATOM   4527  CD1  ILE B 218      22.008   20.959   16.021   1.00 19.55        B
ATOM   4528  C    ILE B 218      22.333   25.745   14.567   1.00 19.93        B
ATOM   4529  O    ILE B 218      23.418   26.145   15.038   1.00 18.55        B
ATOM   4530  N    GLY B 219      21.231   26.488   14.485   1.00 18.45        B
ATOM   4531  CA   GLY B 219      21.173   27.845   14.966   1.00 20.72        B
ATOM   4532  C    GLY B 219      20.213   27.895   16.139   1.00 21.48        B
ATOM   4533  O    GLY B 219      19.724   26.859   16.621   1.00 20.11        B
ATOM   4534  N    SER B 220      19.917   29.104   16.597   1.00 23.01        B
ATOM   4535  CA   SER B 220      19.014   29.266   17.724   1.00 23.61        B
ATOM   4536  CB   SER B 220      19.009   30.718   18.192   1.00 26.05        B
ATOM   4537  OG   SER B 220      18.517   31.556   17.166   1.00 29.78        B
ATOM   4538  C    SER B 220      17.593   28.866   17.345   1.00 23.25        B
ATOM   4539  O    SER B 220      16.825   28.449   18.203   1.00 21.92        B
ATOM   4540  N    ASN B 221      17.240   28.989   16.068   1.00 21.87        B
ATOM   4541  CA   ASN B 221      15.879   28.662   15.667   1.00 21.62        B
ATOM   4542  CB   ASN B 221      15.065   29.948   15.549   1.00 25.88        B
ATOM   4543  CG   ASN B 221      15.037   30.730   16.850   1.00 30.93        B
ATOM   4544  OD1  ASN B 221      15.890   31.585   17.095   1.00 35.31        B
ATOM   4545  ND2  ASN B 221      14.067   30.423   17.700   1.00 32.95        B
ATOM   4546  C    ASN B 221      15.750   27.880   14.378   1.00 18.27        B
ATOM   4547  O    ASN B 221      14.657   27.787   13.830   1.00 18.70        B
ATOM   4548  N    ASN B 222      16.844   27.284   13.919   1.00 18.16        B
ATOM   4549  CA   ASN B 222      16.822   26.555   12.653   1.00 16.52        B
ATOM   4550  CB   ASN B 222      17.258   27.445   11.472   1.00 19.66        B
ATOM   4551  CG   ASN B 222      16.359   28.636   11.258   1.00 21.30        B
ATOM   4552  OD1  ASN B 222      16.377   29.589   12.038   1.00 23.15        B
ATOM   4553  ND2  ASN B 222      15.570   28.607   10.172   1.00 22.47        B
ATOM   4554  C    ASN B 222      17.820   25.447   12.674   1.00 15.05        B
ATOM   4555  O    ASN B 222      18.762   25.461   13.464   1.00 15.87        B
ATOM   4556  N    ILE B 223      17.571   24.457   11.836   1.00 14.78        B
ATOM   4557  CA   ILE B 223      18.531   23.373   11.657   1.00 13.60        B
ATOM   4558  CB   ILE B 223      18.077   22.036   12.294   1.00 13.56        B
ATOM   4559  CG2  ILE B 223      16.722   21.592   11.714   1.00 14.77        B
ATOM   4560  CG1  ILE B 223      19.172   20.962   12.069   1.00 15.05        B
ATOM   4561  CD1  ILE B 223      18.996   19.763   13.023   1.00 17.92        B
ATOM   4562  C    ILE B 223      18.638   23.212   10.158   1.00 15.44        B
ATOM   4563  O    ILE B 223      17.641   23.372    9.433   1.00 15.61        B
ATOM   4564  N    ARG B 224      19.860   22.950    9.685   1.00 15.47        B
ATOM   4565  CA   ARG B 224      20.103   22.744    8.267   1.00 14.89        B
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Figure 1 (continued 46)

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ATOM   4566  CB   ARG B 224    20.845  23.962   7.665  1.00  15.96    B
ATOM   4567  CG   ARG B 224    21.308  23.736   6.237  1.00  17.14    B
ATOM   4568  CD   ARG B 224    21.764  25.058   5.624  1.00  19.60    B
ATOM   4569  NE   ARG B 224    20.628  25.953   5.409  1.00  21.62    B
ATOM   4570  CZ   ARG B 224    20.704  27.193   4.920  1.00  25.09    B
ATOM   4571  NH1  ARG B 224    21.882  27.726   4.589  1.00  26.00    B
ATOM   4572  NH2  ARG B 224    19.594  27.897   4.739  1.00  25.58    B
ATOM   4573  C    ARG B 224    20.936  21.495   8.092  1.00  14.76    B
ATOM   4574  O    ARG B 224    21.838  21.212   8.896  1.00  16.22    B
ATOM   4575  N    ALA B 225    20.611  20.724   7.070  1.00  13.02    B
ATOM   4576  CA   ALA B 225    21.362  19.518   6.742  1.00  15.06    B
ATOM   4577  CB   ALA B 225    20.566  18.273   7.054  1.00  14.63    B
ATOM   4578  C    ALA B 225    21.717  19.524   5.269  1.00  16.06    B
ATOM   4579  O    ALA B 225    20.865  19.761   4.399  1.00  15.83    B
ATOM   4580  N    HIS B 226    22.982  19.229   4.992  1.00  16.22    B
ATOM   4581  CA   HIS B 226    23.470  19.183   3.609  1.00  16.96    B
ATOM   4582  CB   HIS B 226    24.703  20.072   3.438  1.00  20.34    B
ATOM   4583  CG   HIS B 226    24.570  21.455   3.984  1.00  22.82    B
ATOM   4584  CD2  HIS B 226    24.412  21.911   5.251  1.00  25.71    B
ATOM   4585  ND1  HIS B 226    24.731  22.573   3.193  1.00  26.34    B
ATOM   4586  CE1  HIS B 226    24.685  23.657   3.947  1.00  25.51    B
ATOM   4587  NE2  HIS B 226    24.494  23.283   5.199  1.00  26.67    B
ATOM   4588  C    HIS B 226    23.928  17.756   3.288  1.00  17.69    B
ATOM   4589  O    HIS B 226    24.739  17.195   4.031  1.00  18.01    B
ATOM   4590  N    VAL B 227    23.420  17.177   2.203  1.00  16.43    B
ATOM   4591  CA   VAL B 227    23.829  15.846   1.744  1.00  18.02    B
ATOM   4592  CB   VAL B 227    22.774  14.737   2.032  1.00  21.51    B
ATOM   4593  CG1  VAL B 227    23.362  13.373   1.650  1.00  22.64    B
ATOM   4594  CG2  VAL B 227    22.335  14.777   3.508  1.00  24.44    B
ATOM   4595  C    VAL B 227    23.944  15.953   0.236  1.00  18.76    B
ATOM   4596  O    VAL B 227    22.966  16.286  -0.433  1.00  17.98    B
ATOM   4597  N    GLY B 228    25.117  15.673  -0.323  1.00  18.52    B
ATOM   4598  CA   GLY B 228    25.233  15.764  -1.768  1.00  18.19    B
ATOM   4599  C    GLY B 228    24.830  17.146  -2.244  1.00  17.69    B
ATOM   4600  O    GLY B 228    25.267  18.161  -1.704  1.00  17.83    B
ATOM   4601  N    ASP B 229    23.945  17.180  -3.231  1.00  17.92    B
ATOM   4602  CA   ASP B 229    23.548  18.464  -3.754  1.00  17.89    B
ATOM   4603  CB   ASP B 229    23.598  18.416  -5.278  1.00  20.23    B
ATOM   4604  CG   ASP B 229    25.018  18.203  -5.796  1.00  24.39    B
ATOM   4605  OD1  ASP B 229    25.930  18.937  -5.365  1.00  27.15    B
ATOM   4606  OD2  ASP B 229    25.218  17.308  -6.638  1.00  28.68    B
ATOM   4607  C    ASP B 229    22.202  18.935  -3.259  1.00  17.01    B
ATOM   4608  O    ASP B 229    21.532  19.734  -3.937  1.00  16.40    B
ATOM   4609  N    PHE B 230    21.841  18.485  -2.052  1.00  15.16    B
ATOM   4610  CA   PHE B 230    20.563  18.856  -1.404  1.00  16.26    B
ATOM   4611  CB   PHE B 230    19.715  17.622  -1.099  1.00  15.55    B
ATOM   4612  CG   PHE B 230    19.207  16.943  -2.294  1.00  21.50    B
ATOM   4613  CD1  PHE B 230    18.078  17.408  -2.938  1.00  21.49    B
ATOM   4614  CD2  PHE B 230    19.857  15.839  -2.794  1.00  21.72    B
ATOM   4615  CE1  PHE B 230    17.605  16.756  -4.093  1.00  22.44    B
ATOM   4616  CE2  PHE B 230    19.390  15.186  -3.940  1.00  24.25    B
ATOM   4617  CZ   PHE B 230    18.278  15.638  -4.582  1.00  19.43    B
ATOM   4618  C    PHE B 230    20.816  19.547  -0.102  1.00  15.83    B
ATOM   4619  O    PHE B 230    21.745  19.203   0.624  1.00  16.68    B
ATOM   4620  N    ILE B 231    20.006  20.559   0.185  1.00  15.42    B
ATOM   4621  CA   ILE B 231    20.125  21.288   1.419  1.00  15.06    B
ATOM   4622  CB   ILE B 231    20.658  22.707   1.197  1.00  17.17    B
ATOM   4623  CG2  ILE B 231    20.842  23.403   2.547  1.00  17.21    B
ATOM   4624  CG1  ILE B 231    21.945  22.641   0.378  1.00  19.39    B
ATOM   4625  CD1  ILE B 231    23.020  21.819   0.992  1.00  27.13    B
ATOM   4626  C    ILE B 231    18.737  21.413   2.019  1.00  16.11    B
ATOM   4627  O    ILE B 231    17.839  22.016   1.414  1.00  16.41    B
ATOM   4628  N    PHE B 232    18.564  20.830   3.196  1.00  13.24    B
ATOM   4629  CA   PHE B 232    17.287  20.911   3.881  1.00  13.91    B
ATOM   4630  CB   PHE B 232    16.906  19.529   4.423  1.00  13.73    B
ATOM   4631  CG   PHE B 232    15.697  19.553   5.287  1.00  15.40    B
ATOM   4632  CD1  PHE B 232    14.469  19.868   4.725  1.00  15.78    B
ATOM   4633  CD2  PHE B 232    15.785  19.281   6.642  1.00  16.56    B
ATOM   4634  CE1  PHE B 232    13.307  19.911   5.522  1.00  18.04    B
ATOM   4635  CE2  PHE B 232    14.635  19.317   7.459  1.00  18.76    B
ATOM   4636  CZ   PHE B 232    13.398  19.629   6.892  1.00  16.42    B
ATOM   4637  C    PHE B 232    17.399  21.890   5.056  1.00  13.92    B
ATOM   4638  O    PHE B 232    18.365  21.849   5.819  1.00  13.17    B
ATOM   4639  N    THR B 233    16.421  22.790   5.219  1.00  12.41    B
ATOM   4640  CA   THR B 233    16.459  23.718   6.340  1.00  12.88    B
ATOM   4641  CB   THR B 233    16.768  25.163   5.894  1.00  14.92    B
ATOM   4642  OG1  THR B 233    17.997  25.186   5.150  1.00  16.97    B
ATOM   4643  CG2  THR B 233    16.957  26.045   7.122  1.00  15.17    B
ATOM   4644  C    THR B 233    15.097  23.743   7.014  1.00  15.12    B
ATOM   4645  O    THR B 233    14.086  23.800   6.338  1.00  15.11    B
ATOM   4646  N    SER B 234    15.058  23.682   8.343  1.00  14.12    B
ATOM   4647  CA   SER B 234    13.752  23.754   9.028  1.00  14.24    B
ATOM   4648  CB   SER B 234    13.345  22.386   9.589  1.00  14.75    B
ATOM   4649  OG   SER B 234    12.065  22.447  10.269  1.00  15.57    B
ATOM   4650  C    SER B 234    13.799  24.697  10.218  1.00  15.61    B
ATOM   4651  O    SER B 234    14.848  24.856  10.875  1.00  15.62    B
ATOM   4652  N    LYS B 235    12.668  25.318  10.511  1.00  15.65    B
ATOM   4653  CA   LYS B 235    12.614  26.103  11.724  1.00  16.12    B
ATOM   4654  CB   LYS B 235    11.399  27.058  11.698  1.00  20.85    B
ATOM   4655  CG   LYS B 235    11.492  28.066  10.552  1.00  22.12    B
ATOM   4656  CD   LYS B 235    10.989  29.480  10.902  1.00  29.55    B
ATOM   4657  CE   LYS B 235     9.573  29.464  11.445  1.00  31.45    B
ATOM   4658  NZ   LYS B 235     8.906  30.815  11.360  1.00  30.18    B
ATOM   4659  C    LYS B 235    12.482  25.057  12.855  1.00  14.05    B
ATOM   4660  O    LYS B 235    11.991  23.940  12.643  1.00  16.41    B
ATOM   4661  N    LEU B 236    12.945  25.430  14.044  1.00  15.37    B
ATOM   4662  CA   LEU B 236    12.882  24.571  15.220  1.00  15.37    B
ATOM   4663  CB   LEU B 236    14.087  24.837  16.110  1.00  15.88    B
ATOM   4664  CG   LEU B 236    15.463  24.474  15.507  1.00  15.11    B
ATOM   4665  CD1  LEU B 236    16.608  24.944  16.431  1.00  16.66    B
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Figure 1 (continued 47)

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ATOM   4666  CD2  LEU B 236     15.474  22.974  15.228  1.00 16.38      B
ATOM   4667  C    LEU B 236     11.594  24.879  15.982  1.00 18.39      B
ATOM   4668  O    LEU B 236     10.986  25.947  15.802  1.00 19.38      B
ATOM   4669  N    VAL B 237     11.185  23.941  16.831  1.00 21.05      B
ATOM   4670  CA   VAL B 237      9.983  24.091  17.638  1.00 23.90      B
ATOM   4671  CB   VAL B 237      9.278  22.707  17.848  1.00 24.44      B
ATOM   4672  CG1  VAL B 237      8.085  22.831  18.837  1.00 25.05      B
ATOM   4673  CG2  VAL B 237      8.774  22.189  16.503  1.00 26.22      B
ATOM   4674  C    VAL B 237     10.380  24.655  19.000  1.00 26.41      B
ATOM   4675  O    VAL B 237     11.366  24.235  19.589  1.00 25.35      B
ATOM   4676  N    ASP B 238      9.639  25.636  19.496  1.00 32.01      B
ATOM   4677  CA   ASP B 238      9.975  26.158  20.816  1.00 37.53      B
ATOM   4678  CB   ASP B 238      9.528  27.603  20.977  1.00 40.37      B
ATOM   4679  CG   ASP B 238     10.234  28.530  20.022  1.00 42.20      B
ATOM   4680  OD1  ASP B 238     11.453  28.325  19.791  1.00 43.09      B
ATOM   4681  OD2  ASP B 238      9.571  29.466  19.514  1.00 45.01      B
ATOM   4682  C    ASP B 238      9.284  25.302  21.852  1.00 39.40      B
ATOM   4683  O    ASP B 238      8.449  24.457  21.519  1.00 41.81      B
ATOM   4684  N    GLY B 239      9.638  25.498  23.111  1.00 41.31      B
ATOM   4685  CA   GLY B 239      9.004  24.722  24.157  1.00 42.54      B
ATOM   4686  C    GLY B 239     10.019  24.022  25.019  1.00 43.17      B
ATOM   4687  O    GLY B 239     11.188  23.944  24.665  1.00 42.73      B
ATOM   4688  N    ARG B 240      9.572  23.506  26.156  1.00 44.77      B
ATOM   4689  CA   ARG B 240     10.473  22.812  27.062  1.00 45.41      B
ATOM   4690  CB   ARG B 240     10.215  23.260  28.497  1.00 47.67      B
ATOM   4691  CG   ARG B 240      8.807  22.985  28.997  1.00 50.38      B
ATOM   4692  CD   ARG B 240      8.662  23.521  30.408  1.00 52.39      B
ATOM   4693  NE   ARG B 240      8.988  24.942  30.464  1.00 53.18      B
ATOM   4694  CZ   ARG B 240      9.345  25.580  31.572  1.00 54.35      B
ATOM   4695  NH1  ARG B 240      9.422  24.925  32.727  1.00 53.83      B
ATOM   4696  NH2  ARG B 240      9.638  26.871  31.517  1.00 55.03      B
ATOM   4697  C    ARG B 240     10.277  21.306  26.942  1.00 44.25      B
ATOM   4698  O    ARG B 240      9.199  20.790  27.237  1.00 45.09      B
ATOM   4699  N    PHE B 241     11.331  20.615  26.520  1.00 42.31      B
ATOM   4700  CA   PHE B 241     11.290  19.167  26.326  1.00 40.40      B
ATOM   4701  CB   PHE B 241     12.024  18.818  25.019  1.00 37.04      B
ATOM   4702  CG   PHE B 241     11.584  17.518  24.380  1.00 33.05      B
ATOM   4703  CD1  PHE B 241     12.109  16.303  24.798  1.00 32.26      B
ATOM   4704  CD2  PHE B 241     10.666  17.529  23.338  1.00 30.96      B
ATOM   4705  CE1  PHE B 241     11.727  15.108  24.179  1.00 29.39      B
ATOM   4706  CE2  PHE B 241     10.276  16.347  22.714  1.00 29.62      B
ATOM   4707  CZ   PHE B 241     10.814  15.134  23.141  1.00 28.51      B
ATOM   4708  C    PHE B 241     11.892  18.398  27.511  1.00 39.78      B
ATOM   4709  O    PHE B 241     12.919  18.785  28.077  1.00 40.91      B
ATOM   4710  N    PRO B 242     11.254  17.279  27.890  1.00 38.82      B
ATOM   4711  CD   PRO B 242      9.987  16.826  27.286  1.00 37.70      B
ATOM   4712  CA   PRO B 242     11.660  16.404  28.997  1.00 37.16      B
ATOM   4713  CB   PRO B 242     10.688  15.230  28.874  1.00 37.98      B
ATOM   4714  CG   PRO B 242      9.448  15.869  28.336  1.00 37.43      B
ATOM   4715  C    PRO B 242     13.124  15.947  28.987  1.00 36.91      B
ATOM   4716  O    PRO B 242     13.728  15.748  27.925  1.00 35.36      B
ATOM   4717  N    ASP B 243     13.675  15.763  30.184  1.00 35.76      B
ATOM   4718  CA   ASP B 243     15.053  15.323  30.369  1.00 36.57      B
ATOM   4719  CB   ASP B 243     15.625  15.957  31.639  1.00 35.26      B
ATOM   4720  CG   ASP B 243     17.064  15.549  31.907  1.00 36.71      B
ATOM   4721  OD1  ASP B 243     17.556  14.587  31.281  1.00 36.01      B
ATOM   4722  OD2  ASP B 243     17.709  16.188  32.767  1.00 36.91      B
ATOM   4723  C    ASP B 243     15.114  13.796  30.495  1.00 36.45      B
ATOM   4724  O    ASP B 243     14.919  13.251  31.576  1.00 36.71      B
ATOM   4725  N    TYR B 244     15.419  13.103  29.407  1.00 36.69      B
ATOM   4726  CA   TYR B 244     15.477  11.638  29.446  1.00 36.02      B
ATOM   4727  CB   TYR B 244     16.148  11.089  28.186  1.00 34.53      B
ATOM   4728  CG   TYR B 244     17.657  10.998  28.255  1.00 34.00      B
ATOM   4729  CD1  TYR B 244     18.462  12.105  27.968  1.00 32.87      B
ATOM   4730  CE1  TYR B 244     19.858  12.000  27.984  1.00 34.13      B
ATOM   4731  CD2  TYR B 244     18.281   9.791  28.566  1.00 33.14      B
ATOM   4732  CE2  TYR B 244     19.665   9.672  28.581  1.00 34.72      B
ATOM   4733  CZ   TYR B 244     20.449  10.783  28.283  1.00 34.56      B
ATOM   4734  OH   TYR B 244     21.811  10.638  28.235  1.00 36.14      B
ATOM   4735  C    TYR B 244     16.199  11.060  30.673  1.00 37.56      B
ATOM   4736  O    TYR B 244     15.795  10.029  31.215  1.00 36.17      B
ATOM   4737  N    ARG B 245     17.269  11.728  31.092  1.00 38.21      B
ATOM   4738  CA   ARG B 245     18.074  11.296  32.231  1.00 40.14      B
ATOM   4739  CB   ARG B 245     19.166  12.333  32.518  1.00 40.81      B
ATOM   4740  CG   ARG B 245     20.029  12.665  31.319  1.00 43.08      B
ATOM   4741  CD   ARG B 245     21.075  13.731  31.631  1.00 43.61      B
ATOM   4742  NE   ARG B 245     21.787  14.137  30.420  1.00 45.10      B
ATOM   4743  CZ   ARG B 245     21.231  14.807  29.413  1.00 45.50      B
ATOM   4744  NH1  ARG B 245     19.952  15.157  29.464  1.00 44.89      B
ATOM   4745  NH2  ARG B 245     21.956  15.131  28.348  1.00 46.19      B
ATOM   4746  C    ARG B 245     17.233  11.102  33.486  1.00 40.09      B
ATOM   4747  O    ARG B 245     17.574  10.297  34.352  1.00 40.05      B
ATOM   4748  N    ARG B 246     16.133  11.840  33.560  1.00 39.85      B
ATOM   4749  CA   ARG B 246     15.239  11.808  34.707  1.00 40.96      B
ATOM   4750  CB   ARG B 246     14.755  13.227  34.984  1.00 43.17      B
ATOM   4751  CG   ARG B 246     15.880  14.252  35.113  1.00 46.06      B
ATOM   4752  CD   ARG B 246     16.443  14.295  36.529  1.00 47.96      B
ATOM   4753  NE   ARG B 246     15.374  14.318  37.524  1.00 49.96      B
ATOM   4754  CZ   ARG B 246     14.316  15.126  37.477  1.00 50.99      B
ATOM   4755  NH1  ARG B 246     14.169  15.992  36.481  1.00 51.52      B
ATOM   4756  NH2  ARG B 246     13.396  15.067  38.430  1.00 52.32      B
ATOM   4757  C    ARG B 246     14.022  10.889  34.566  1.00 40.13      B
ATOM   4758  O    ARG B 246     13.384  10.536  35.560  1.00 39.22      B
ATOM   4759  N    VAL B 247     13.695  10.532  33.327  1.00 38.72      B
ATOM   4760  CA   VAL B 247     12.553   9.675  33.018  1.00 36.88      B
ATOM   4761  CB   VAL B 247     12.061   9.942  31.585  1.00 37.39      B
ATOM   4762  CG1  VAL B 247     10.930   8.991  31.216  1.00 36.97      B
ATOM   4763  CG2  VAL B 247     11.624  11.391  31.462  1.00 37.68      B
ATOM   4764  C    VAL B 247     12.962   8.218  33.133  1.00 35.57      B
ATOM   4765  O    VAL B 247     12.125   7.334  33.308  1.00 36.36      B
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Figure 1 (continued 48)

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ATOM   4766  N   LEU B 248      14.260   7.974  33.019  1.00 34.36      B
ATOM   4767  CA  LEU B 248      14.797   6.627  33.124  1.00 34.03      B
ATOM   4768  CB  LEU B 248      16.296   6.621  32.855  1.00 33.66      B
ATOM   4769  CG  LEU B 248      16.785   7.109  31.499  1.00 33.85      B
ATOM   4770  CD1 LEU B 248      18.285   6.813  31.398  1.00 34.48      B
ATOM   4771  CD2 LEU B 248      16.017   6.403  30.386  1.00 33.89      B
ATOM   4772  C   LEU B 248      14.564   6.083  34.525  1.00 34.01      B
ATOM   4773  O   LEU B 248      14.860   6.756  35.519  1.00 32.99      B
ATOM   4774  N   PRO B 249      14.038   4.851  34.622  1.00 33.37      B
ATOM   4775  CD  PRO B 249      13.707   3.936  33.514  1.00 32.25      B
ATOM   4776  CA  PRO B 249      13.776   4.221  35.921  1.00 33.57      B
ATOM   4777  CB  PRO B 249      13.565   2.751  35.546  1.00 32.82      B
ATOM   4778  CG  PRO B 249      12.921   2.845  34.210  1.00 32.30      B
ATOM   4779  C   PRO B 249      14.965   4.423  36.875  1.00 33.81      B
ATOM   4780  O   PRO B 249      16.113   4.182  36.514  1.00 31.74      B
ATOM   4781  N   LYS B 250      14.672   4.869  38.091  1.00 36.30      B
ATOM   4782  CA  LYS B 250      15.695   5.128  39.102  1.00 39.83      B
ATOM   4783  CB  LYS B 250      15.024   5.653  40.370  1.00 41.65      B
ATOM   4784  CG  LYS B 250      13.622   6.224  40.144  1.00 44.53      B
ATOM   4785  CD  LYS B 250      12.980   6.637  41.466  1.00 46.40      B
ATOM   4786  CE  LYS B 250      11.562   7.139  41.267  1.00 47.75      B
ATOM   4787  NZ  LYS B 250      10.957   7.618  42.538  1.00 48.54      B
ATOM   4788  C   LYS B 250      16.562   3.912  39.454  1.00 40.80      B
ATOM   4789  O   LYS B 250      17.773   3.915  39.240  1.00 42.14      B
ATOM   4790  N   ASN B 251      15.944   2.881  40.016  1.00 40.30      B
ATOM   4791  CA  ASN B 251      16.687   1.686  40.388  1.00 41.84      B
ATOM   4792  CB  ASN B 251      16.907   1.661  41.899  1.00 43.14      B
ATOM   4793  CG  ASN B 251      17.875   2.734  42.365  1.00 44.47      B
ATOM   4794  OD1 ASN B 251      17.623   3.421  43.353  1.00 45.51      B
ATOM   4795  ND2 ASN B 251      18.996   2.873  41.662  1.00 45.61      B
ATOM   4796  C   ASN B 251      15.976   0.413  39.942  1.00 41.06      B
ATOM   4797  O   ASN B 251      15.388  -0.302  40.754  1.00 40.34      B
ATOM   4798  N   PRO B 252      16.020   0.121  38.634  1.00 40.93      B
ATOM   4799  CD  PRO B 252      16.646   0.951  37.592  1.00 40.87      B
ATOM   4800  CA  PRO B 252      15.384  -1.069  38.051  1.00 40.56      B
ATOM   4801  CB  PRO B 252      15.505  -0.839  36.539  1.00 40.95      B
ATOM   4802  CG  PRO B 252      15.797   0.628  36.393  1.00 41.84      B
ATOM   4803  C   PRO B 252      16.144  -2.323  38.481  1.00 40.59      B
ATOM   4804  O   PRO B 252      16.811  -2.953  37.666  1.00 41.49      B
ATOM   4805  N   ASP B 253      16.024  -2.681  39.754  1.00 39.23      B
ATOM   4806  CA  ASP B 253      16.725  -3.833  40.318  1.00 38.72      B
ATOM   4807  CB  ASP B 253      16.316  -4.011  41.799  1.00 40.83      B
ATOM   4808  CG  ASP B 253      14.803  -4.237  41.995  1.00 42.90      B
ATOM   4809  OD1 ASP B 253      13.992  -3.318  41.739  1.00 44.02      B
ATOM   4810  OD2 ASP B 253      14.412  -5.347  42.423  1.00 44.75      B
ATOM   4811  C   ASP B 253      16.616  -5.183  39.585  1.00 36.72      B
ATOM   4812  O   ASP B 253      17.601  -5.922  39.478  1.00 36.03      B
ATOM   4813  N   LYS B 254      15.432  -5.484  39.066  1.00 32.67      B
ATOM   4814  CA  LYS B 254      15.164  -6.751  38.403  1.00 30.08      B
ATOM   4815  CB  LYS B 254      13.688  -7.106  38.593  1.00 28.89      B
ATOM   4816  CG  LYS B 254      13.194  -7.092  40.049  1.00 29.78      B
ATOM   4817  CD  LYS B 254      11.661  -7.160  40.098  1.00 28.23      B
ATOM   4818  CE  LYS B 254      11.120  -7.160  41.515  1.00 33.00      B
ATOM   4819  NZ  LYS B 254      11.584  -5.968  42.297  1.00 33.49      B
ATOM   4820  C   LYS B 254      15.489  -6.736  36.912  1.00 29.93      B
ATOM   4821  O   LYS B 254      14.811  -6.060  36.135  1.00 30.36      B
ATOM   4822  N   HIS B 255      16.495  -7.501  36.519  1.00 27.24      B
ATOM   4823  CA  HIS B 255      16.897  -7.564  35.118  1.00 26.91      B
ATOM   4824  CB  HIS B 255      18.402  -7.339  34.966  1.00 30.35      B
ATOM   4825  CG  HIS B 255      18.876  -6.000  35.429  1.00 33.70      B
ATOM   4826  CD2 HIS B 255      20.129  -5.522  35.617  1.00 34.19      B
ATOM   4827  ND1 HIS B 255      18.021  -4.950  35.695  1.00 35.10      B
ATOM   4828  CE1 HIS B 255      18.730  -3.882  36.025  1.00 35.55      B
ATOM   4829  NE2 HIS B 255      20.011  -4.204  35.986  1.00 34.99      B
ATOM   4830  C   HIS B 255      16.587  -8.885  34.453  1.00 24.52      B
ATOM   4831  O   HIS B 255      16.979  -9.935  34.936  1.00 23.10      B
ATOM   4832  N   LEU B 256      15.923  -8.824  33.307  1.00 22.74      B
ATOM   4833  CA  LEU B 256      15.606 -10.014  32.551  1.00 21.40      B
ATOM   4834  CB  LEU B 256      14.080 -10.157  32.461  1.00 23.90     \B
ATOM   4835  CG  LEU B 256      13.435 -11.154  31.508  1.00 24.90     \B
ATOM   4836  CD1 LEU B 256      12.064 -11.555  32.033  1.00 26.89      B
ATOM   4837  CD2 LEU B 256      13.322 -10.514  30.136  1.00 23.55      B
ATOM   4838  C   LEU B 256      16.210  -9.867  31.154  1.00 19.61      B
ATOM   4839  O   LEU B 256      16.191  -8.768  30.581  1.00 18.29      B
ATOM   4840  N   GLU B 257      16.774 -10.955  30.641  1.00 18.37      B
ATOM   4841  CA  GLU B 257      17.329 -10.973  29.287  1.00 18.54      B
ATOM   4842  CB  GLU B 257      18.848 -11.229  29.318  1.00 21.51      B
ATOM   4843  CG  GLU B 257      19.681 -10.093  29.921  1.00 27.65      B
ATOM   4844  CD  GLU B 257      19.758 -10.132 -31.460  1.00 31.19      B
ATOM   4845  OE1 GLU B 257      19.940 -11.236  32.023  1.00 33.27      B
ATOM   4846  OE2 GLU B 257      19.664  -9.056  32.108  1.00 32.03      B
ATOM   4847  C   GLU B 257      16.616 -12.085  28.510  1.00 17.69      B
ATOM   4848  O   GLU B 257      16.374 -13.182  29.042  1.00 18.75      B
ATOM   4849  N   ALA B 258      16.262 -11.808  27.256  1.00 17.24      B
ATOM   4850  CA  ALA B 258      15.558 -12.786  26.423  1.00 18.43      B
ATOM   4851  CB  ALA B 258      14.079 -12.680  26.654  1.00 22.18      B
ATOM   4852  C   ALA B 258      15.840 -12.507  24.966  1.00 19.20      B
ATOM   4853  O   ALA B 258      16.180 -11.370  24.609  1.00 19.32      B
ATOM   4854  N   GLY B 259      15.713 -13.539  24.130  1.00 18.97      B
ATOM   4855  CA  GLY B 259      15.917 -13.346  22.700  1.00 18.87      B
ATOM   4856  C   GLY B 259      14.894 -12.358  22.161  1.00 19.04      B
ATOM   4857  O   GLY B 259      13.693 -12.468  22.453  1.00 18.24      B
ATOM   4858  N   CYS B 260      15.356 -11.389  21.375  1.00 17.25      B
ATOM   4859  CA  CYS B 260      14.439 -10.387  20.846  1.00 18.30      B
ATOM   4860  CB  CYS B 260      15.216  -9.341  20.048  1.00 17.26      B
ATOM   4861  SG  CYS B 260      14.169  -7.950  19.540  1.00 23.04      B
ATOM   4862  C   CYS B 260      13.335 -10.980  19.981  1.00 17.67      B
ATOM   4863  O   CYS B 260      12.164 -10.678  20.188  1.00 18.38      B
ATOM   4864  N   ASP B 261      13.694 -11.811  19.006  1.00 18.04      B
ATOM   4865  CA  ASP B 261      12.666 -12.364  18.140  1.00 18.32      B
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Figure 1 (continued 49)

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ATOM   4866   CB   ASP B 261    13.290 -13.046  16.919  1.00 21.68      B
ATOM   4867   CG   ASP B 261    12.334 -13.065  15.738  1.00 24.40      B
ATOM   4868   OD1  ASP B 261    11.951 -14.160  15.306  1.00 27.81      B
ATOM   4869   OD2  ASP B 261    11.957 -11.968  15.252  1.00 29.16      B
ATOM   4870   C    ASP B 261    11.685 -13.311  18.828  1.00 16.90      B
ATOM   4871   O    ASP B 261    10.480 -13.263  18.540  1.00 17.30      B
ATOM   4872   N    LEU B 262    12.154 -14.159  19.737  1.00 14.56      B
ATOM   4873   CA   LEU B 262    11.191 -15.037  20.412  1.00 17.35      B
ATOM   4874   CB   LEU B 262    11.872 -16.053  21.329  1.00 19.61      B
ATOM   4875   CG   LEU B 262    12.472 -17.269  20.618  1.00 19.99      B
ATOM   4876   CD1  LEU B 262    13.259 -18.057  21.656  1.00 21.84      B
ATOM   4877   CD2  LEU B 262    11.395 -18.129  19.939  1.00 21.69      B
ATOM   4878   C    LEU B 262    10.248 -14.170  21.243  1.00 15.38      B
ATOM   4879   O    LEU B 262     9.065 -14.433  21.311  1.00 15.79      B
ATOM   4880   N    LEU B 263    10.780 -13.136  21.892  1.00 15.25      B
ATOM   4881   CA   LEU B 263     9.923 -12.288  22.713  1.00 16.20      B
ATOM   4882   CB   LEU B 263    10.795 -11.293  23.487  1.00 18.03      B
ATOM   4883   CG   LEU B 263    10.111 -10.421  24.532  1.00 21.36      B
ATOM   4884   CD1  LEU B 263     9.540 -11.366  25.608  1.00 21.04      B
ATOM   4885   CD2  LEU B 263    11.103  -9.396  25.155  1.00 22.83      B
ATOM   4886   C    LEU B 263     8.916 -11.546  21.826  1.00 16.77      B
ATOM   4887   O    LEU B 263     7.735 -11.457  22.133  1.00 15.34      B
ATOM   4888   N    LYS B 264     9.395 -11.034  20.711  1.00 16.41      B
ATOM   4889   CA   LYS B 264     8.525 -10.302  19.806  1.00 16.03      B
ATOM   4890   CB   LYS B 264     9.335  -9.738  18.636  1.00 18.07      B
ATOM   4891   CG   LYS B 264     8.475  -9.099  17.595  1.00 22.20      B
ATOM   4892   CD   LYS B 264     9.281  -8.250  16.610  1.00 26.37      B
ATOM   4893   CE   LYS B 264    10.346  -9.023  15.870  1.00 28.03      B
ATOM   4894   NZ   LYS B 264    11.318  -8.076  15.214  1.00 31.01      B
ATOM   4895   C    LYS B 264     7.412 -11.191  19.262  1.00 15.79      B
ATOM   4896   O    LYS B 264     6.236 -10.796  19.245  1.00 14.64      B
ATOM   4897   N    GLN B 265     7.784 -12.391  18.817  1.00 15.72      B
ATOM   4898   CA   GLN B 265     6.779 -13.286  18.244  1.00 16.84      B
ATOM   4899   CB   GLN B 265     7.435 -14.519  17.598  1.00 17.09      B
ATOM   4900   CG   GLN B 265     8.320 -14.204  16.357  1.00 18.42      B
ATOM   4901   CD   GLN B 265     7.782 -13.068  15.479  1.00 22.54      B
ATOM   4902   OE1  GLN B 265     6.570 -12.890  15.303  1.00 26.47      B
ATOM   4903   NE2  GLN B 265     8.704 -12.294  14.913  1.00 25.44      B
ATOM   4904   C    GLN B 265     5.753 -13.721  19.293  1.00 14.97      B
ATOM   4905   O    GLN B 265     4.572 -13.896  18.984  1.00 15.81      B
ATOM   4906   N    ALA B 266     6.185 -13.892  20.535  1.00 15.47      B
ATOM   4907   CA   ALA B 266     5.255 -14.301  21.598  1.00 14.14      B
ATOM   4908   CB   ALA B 266     6.022 -14.664  22.883  1.00 15.40      B
ATOM   4909   C    ALA B 266     4.283 -13.174  21.879  1.00 15.29      B
ATOM   4910   O    ALA B 266     3.083 -13.405  22.019  1.00 13.58      B
ATOM   4911   N    PHE B 267     4.807 -11.951  21.974  1.00 13.20      B
ATOM   4912   CA   PHE B 267     3.921 -10.801  22.218  1.00 13.52      B
ATOM   4913   CB   PHE B 267     4.744  -9.513  22.439  1.00 13.38      B
ATOM   4914   CG   PHE B 267     5.198  -9.317  23.868  1.00 13.24      B
ATOM   4915   CD1  PHE B 267     4.271  -9.194  24.912  1.00 14.43      B
ATOM   4916   CD2  PHE B 267     6.565  -9.244  24.169  1.00 14.23      B
ATOM   4917   CE1  PHE B 267     4.694  -8.992  26.240  1.00 16.33      B
ATOM   4918   CE2  PHE B 267     6.986  -9.048  25.487  1.00 16.29      B
ATOM   4919   CZ   PHE B 267     6.051  -8.920  26.516  1.00 15.41      B
ATOM   4920   C    PHE B 267     2.960 -10.609  21.038  1.00 14.30      B
ATOM   4921   O    PHE B 267     1.788 -10.261  21.248  1.00 14.42      B
ATOM   4922   N    ALA B 268     3.446 -10.818  19.813  1.00 14.41      B
ATOM   4923   CA   ALA B 268     2.630 -10.628  18.615  1.00 15.14      B
ATOM   4924   CB   ALA B 268     3.504 -10.794  17.379  1.00 14.71      B
ATOM   4925   C    ALA B 268     1.480 -11.633  18.606  1.00 14.93      B
ATOM   4926   O    ALA B 268     0.329 -11.286  18.247  1.00 14.13      B
ATOM   4927   N    ARG B 269     1.757 -12.880  19.008  1.00 13.12      B
ATOM   4928   CA   ARG B 269     0.671 -13.840  19.015  1.00 13.27      B
ATOM   4929   CB   ARG B 269     1.214 -15.269  19.154  1.00 14.61      B
ATOM   4930   CG   ARG B 269     1.831 -15.845  17.872  1.00 13.63      B
ATOM   4931   CD   ARG B 269     2.204 -17.358  18.026  1.00 13.98      B
ATOM   4932   NE   ARG B 269     3.118 -17.555  19.133  1.00 13.12      B
ATOM   4933   CZ   ARG B 269     4.448 -17.518  19.033  1.00 15.76      B
ATOM   4934   NH1  ARG B 269     5.034 -17.313  17.853  1.00 14.76      B
ATOM   4935   NH2  ARG B 269     5.201 -17.683  20.114  1.00 14.02      B
ATOM   4936   C    ARG B 269    -0.324 -13.530  20.153  1.00 14.05      B
ATOM   4937   O    ARG B 269    -1.546 -13.617  19.952  1.00 14.17      B
ATOM   4938   N    ALA B 270     0.191 -13.167  21.338  1.00 13.89      B
ATOM   4939   CA   ALA B 270    -0.687 -12.886  22.471  1.00 14.30      B
ATOM   4940   CB   ALA B 270     0.141 -12.603  23.735  1.00 13.36      B
ATOM   4941   C    ALA B 270    -1.568 -11.682  22.159  1.00 13.96      B
ATOM   4942   O    ALA B 270    -2.748 -11.645  22.542  1.00 15.55      B
ATOM   4943   N    ALA B 271    -1.002 -10.720  21.438  1.00 14.27      B
ATOM   4944   CA   ALA B 271    -1.726  -9.500  21.096  1.00 13.67      B
ATOM   4945   CB   ALA B 271    -0.836  -8.599  20.291  1.00 15.13      B
ATOM   4946   C    ALA B 271    -3.002  -9.795  20.333  1.00 15.03      B
ATOM   4947   O    ALA B 271    -3.972  -9.041  20.421  1.00 15.64      B
ATOM   4948   N    ILE B 272    -3.016 -10.898  19.595  1.00 14.65      B
ATOM   4949   CA   ILE B 272    -4.196 -11.249  18.821  1.00 15.22      B
ATOM   4950   CB   ILE B 272    -3.974 -12.585  18.079  1.00 13.73      B
ATOM   4951   CG2  ILE B 272    -5.242 -13.018  17.334  1.00 15.77      B
ATOM   4952   CG1  ILE B 272    -2.854 -12.439  17.060  1.00 15.68      B
ATOM   4953   CD1  ILE B 272    -2.364 -13.817  16.555  1.00 16.71      B
ATOM   4954   C    ILE B 272    -5.430 -11.343  19.725  1.00 16.21      B
ATOM   4955   O    ILE B 272    -6.524 -10.941  19.311  1.00 16.96      B
ATOM   4956   N    LEU B 273    -5.277 -11.870  20.949  1.00 16.13      B
ATOM   4957   CA   LEU B 273    -6.425 -11.991  21.858  1.00 15.61      B
ATOM   4958   CB   LEU B 273    -6.508 -13.415  22.449  1.00 16.11      B
ATOM   4959   CG   LEU B 273    -6.563 -14.492  21.330  1.00 16.18      B
ATOM   4960   CD1  LEU B 273    -6.548 -15.891  21.960  1.00 16.52      B
ATOM   4961   CD2  LEU B 273    -7.847 -14.316  20.469  1.00 18.42      B
ATOM   4962   C    LEU B 273    -6.473 -10.946  22.968  1.00 17.30      B
ATOM   4963   O    LEU B 273    -7.106 -11.158  23.997  1.00 17.88      B
ATOM   4964   N    SER B 274    -5.811  -9.809  22.742  1.00 17.24      B
ATOM   4965   CA   SER B 274    -5.863  -8.708  23.702  1.00 18.02      B
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Figure 1 (continued 50)

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ATOM   4966  CB   SER B 274    -4.556  -7.906  23.686  1.00 17.37       B
ATOM   4967  OG   SER B 274    -4.390  -7.180  22.474  1.00 17.38       B
ATOM   4968  C    SER B 274    -7.033  -7.796  23.318  1.00 17.71       B
ATOM   4969  O    SER B 274    -7.542  -7.858  22.189  1.00 17.27       B
ATOM   4970  N    ASN B 275    -7.464  -6.965  24.260  1.00 17.56       B
ATOM   4971  CA   ASN B 275    -8.550  -6.014  24.026  1.00 18.55       B
ATOM   4972  CB   ASN B 275    -8.705  -5.145  25.269  1.00 17.80       B
ATOM   4973  CG   ASN B 275    -9.904  -4.223  25.180  1.00 19.42       B
ATOM   4974  OD1  ASN B 275    -9.934  -3.339  24.331  1.00 19.77       B
ATOM   4975  ND2  ASN B 275   -10.898  -4.431  26.063  1.00 22.03       B
ATOM   4976  C    ASN B 275    -8.184  -5.166  22.792  1.00 20.76       B
ATOM   4977  O    ASN B 275    -7.090  -4.585  22.723  1.00 17.98       B
ATOM   4978  N    GLU B 276    -9.091  -5.093  21.816  1.00 21.76       B
ATOM   4979  CA   GLU B 276    -8.779  -4.365  20.591  1.00 23.72       B
ATOM   4980  CB   GLU B 276    -9.897  -4.556  19.554  1.00 25.43       B
ATOM   4981  CG   GLU B 276    -9.852  -5.932  18.891  1.00 29.37       B
ATOM   4982  CD   GLU B 276   -11.021  -6.196  17.960  1.00 32.27       B
ATOM   4983  OE1  GLU B 276   -11.600  -5.217  17.442  1.00 33.37       B
ATOM   4984  OE2  GLU B 276   -11.348  -7.390  17.745  1.00 32.65       B
ATOM   4985  C    GLU B 276    -8.481  -2.888  20.782  1.00 23.01       B
ATOM   4986  O    GLU B 276    -7.749  -2.292  19.986  1.00 23.94       B
ATOM   4987  N    LYS B 277    -9.034  -2.310  21.837  1.00 23.05       B
ATOM   4988  CA   LYS B 277    -8.810  -0.910  22.113  1.00 23.82       B
ATOM   4989  CB   LYS B 277   -10.085  -0.230  22.638  1.00 25.13       B
ATOM   4990  CG   LYS B 277    -9.852   1.262  22.949  1.00 28.98       B
ATOM   4991  CD   LYS B 277   -11.084   2.016  23.463  1.00 31.73       B
ATOM   4992  CE   LYS B 277   -10.744   3.512  23.598  1.00 33.68       B
ATOM   4993  NZ   LYS B 277   -11.577   4.222  24.623  1.00 35.35       B
ATOM   4994  C    LYS B 277    -7.681  -0.655  23.104  1.00 23.58       B
ATOM   4995  O    LYS B 277    -6.790   0.162  22.825  1.00 23.95       B
ATOM   4996  N    PHE B 278    -7.702  -1.352  24.244  1.00 21.16       B
ATOM   4997  CA   PHE B 278    -6.698  -1.155  25.300  1.00 20.62       B
ATOM   4998  CB   PHE B 278    -7.318  -1.432  26.663  1.00 21.99       B
ATOM   4999  CG   PHE B 278    -8.431  -0.459  27.021  1.00 26.60       B
ATOM   5000  CD1  PHE B 278    -8.142   0.882  27.268  1.00 29.14       B
ATOM   5001  CD2  PHE B 278    -9.760  -0.869  27.021  1.00 28.88       B
ATOM   5002  CE1  PHE B 278    -9.177   1.816  27.508  1.00 30.11       B
ATOM   5003  CE2  PHE B 278   -10.795   0.052  27.258  1.00 30.65       B
ATOM   5004  CZ   PHE B 278   -10.496   1.391  27.500  1.00 30.56       B
ATOM   5005  C    PHE B 278    -5.403  -1.957  25.131  1.00 19.25       B
ATOM   5006  O    PHE B 278    -4.356  -1.582  25.677  1.00 18.94       B
ATOM   5007  N    ARG B 279    -5.484  -3.045  24.371  1.00 19.60       B
ATOM   5008  CA   ARG B 279    -4.307  -3.865  24.050  1.00 18.45       B
ATOM   5009  CB   ARG B 279    -3.404  -3.067  23.088  1.00 19.81       B
ATOM   5010  CG   ARG B 279    -4.078  -2.674  21.767  1.00 19.94       B
ATOM   5011  CD   ARG B 279    -4.097  -3.843  20.776  1.00 21.13       B
ATOM   5012  NE   ARG B 279    -2.777  -3.988  20.175  1.00 23.76       B
ATOM   5013  CZ   ARG B 279    -2.423  -4.973  19.365  1.00 22.43       B
ATOM   5014  NH1  ARG B 279    -3.297  -5.921  19.058  1.00 25.01       B
ATOM   5015  NH2  ARG B 279    -1.202  -4.987  18.838  1.00 23.93       B
ATOM   5016  C    ARG B 279    -3.460  -4.360  25.210  1.00 18.23       B
ATOM   5017  O    ARG B 279    -2.261  -4.590  25.046  1.00 16.99       B
ATOM   5018  N    GLY B 280    -4.062  -4.589  26.365  1.00 16.92       B
ATOM   5019  CA   GLY B 280    -3.260  -5.011  27.491  1.00 15.52       B
ATOM   5020  C    GLY B 280    -2.864  -6.477  27.534  1.00 14.43       B
ATOM   5021  O    GLY B 280    -3.652  -7.360  27.199  1.00 15.18       B
ATOM   5022  N    VAL B 281    -1.623  -6.709  27.942  1.00 15.08       B
ATOM   5023  CA   VAL B 281    -1.104  -8.062  28.125  1.00 14.23       B
ATOM   5024  CB   VAL B 281    -0.046  -8.473  27.057  1.00 12.60       B
ATOM   5025  CG1  VAL B 281    -0.707  -8.654  25.727  1.00 17.31       B
ATOM   5026  CG2  VAL B 281     1.061  -7.440  26.981  1.00 15.23       B
ATOM   5027  C    VAL B 281    -0.450  -8.059  29.497  1.00 13.94       B
ATOM   5028  O    VAL B 281    -0.049  -7.000  30.034  1.00 14.27       B
ATOM   5029  N    ARG B 282    -0.387  -9.241  30.091  1.00 12.68       B
ATOM   5030  CA   ARG B 282     0.202  -9.381  31.405  1.00 14.01       B
ATOM   5031  CB   ARG B 282    -0.753 -10.142  32.337  1.00 18.49       B
ATOM   5032  CG   ARG B 282    -1.999  -9.373  32.712  1.00 25.67       B
ATOM   5033  CD   ARG B 282    -2.770 -10.154  33.784  1.00 31.13       B
ATOM   5034  NE   ARG B 282    -3.601  -9.274  34.606  1.00 36.93      )B
ATOM   5035  CZ   ARG B 282    -3.765  -9.449  35.908  1.00 38.95       B
ATOM   5036  NH1  ARG B 282    -3.154 -10.470  36.510  1.00 41.34       B
ATOM   5037  NH2  ARG B 282    -4.511  -8.605  36.615  1.00 42.07       B
ATOM   5038  C    ARG B 282     1.489 -10.168  31.273  1.00 13.94       B
ATOM   5039  O    ARG B 282     1.568 -11.118  30.483  1.00 13.78       B
ATOM   5040  N    LEU B 283     2.503  -9.736  32.016  1.00 11.77       B
ATOM   5041  CA   LEU B 283     3.784 -10.427  32.050  1.00 12.94       B
ATOM   5042  CB   LEU B 283     4.931  -9.460  31.806  1.00 13.78       B
ATOM   5043  CG   LEU B 283     5.246  -9.059  30.376  1.00 16.55       B
ATOM   5044  CD1  LEU B 283     4.078  -8.291  29.772  1.00 18.52       B
ATOM   5045  CD2  LEU B 283     6.512  -8.199  30.417  1.00 15.82       B
ATOM   5046  C    LEU B 283     3.989 -10.979  33.454  1.00 13.65       B
ATOM   5047  O    LEU B 283     3.832 -10.232  34.422  1.00 15.26       B
ATOM   5048  N    TYR B 284     4.281 -12.271  33.584  1.00 13.05       B
ATOM   5049  CA   TYR B 284     4.580 -12.809  34.913  1.00 13.63       B
ATOM   5050  CB   TYR B 284     3.686 -14.004  35.283  1.00 13.56       B
ATOM   5051  CG   TYR B 284     3.808 -14.302  36.781  1.00 18.42       B
ATOM   5052  CD1  TYR B 284     2.898 -13.778  37.698  1.00 20.54       B
ATOM   5053  CE1  TYR B 284     3.069 -13.971  39.101  1.00 22.11       B
ATOM   5054  CD2  TYR B 284     4.890 -15.024  37.260  1.00 19.69       B
ATOM   5055  CE2  TYR B 284     5.088 -15.221  38.628  1.00 20.37       B
ATOM   5056  CZ   TYR B 284     4.175 -14.694  39.544  1.00 22.54       B
ATOM   5057  OH   TYR B 284     4.412 -14.897  40.889  1.00 21.81       B
ATOM   5058  C    TYR B 284     6.027 -13.271  34.818  1.00 12.58       B
ATOM   5059  O    TYR B 284     6.357 -14.144  34.026  1.00 13.78       B
ATOM   5060  N    VAL B 285     6.898 -12.675  35.635  1.00 12.36       B
ATOM   5061  CA   VAL B 285     8.306 -12.990  35.601  1.00 13.80       B
ATOM   5062  CB   VAL B 285     9.106 -11.669  35.724  1.00 16.86       B
ATOM   5063  CG1  VAL B 285    10.576 -11.922  35.640  1.00 20.79       B
ATOM   5064  CG2  VAL B 285     8.675 -10.718  34.599  1.00 19.51       B
ATOM   5065  C    VAL B 285     8.656 -13.928  36.761  1.00 12.81       B
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Figure 1 (continued 51)

ATOM	5066	O	VAL	B	285	8.313	-13.643	37.889	1.00	14.44	B
ATOM	5067	N	SER	B	286	9.318	-15.036	36.464	1.00	13.79	B
ATOM	5068	CA	SER	B	286	9.730	-15.996	37.493	1.00	14.29	B
ATOM	5069	CB	SER	B	286	8.716	-17.148	37.609	1.00	14.83	B
ATOM	5070	OG	SER	B	286	8.623	-17.928	36.439	1.00	17.73	B
ATOM	5071	C	SER	B	286	11.145	-16.492	37.139	1.00	14.68	B
ATOM	5072	O	SER	B	286	11.712	-16.116	36.103	1.00	14.34	B
ATOM	5073	N	GLU	B	287	11.732	-17.338	37.971	1.00	15.06	B
ATOM	5074	CA	GLU	B	287	13.112	-17.732	37.692	1.00	16.29	B
ATOM	5075	CB	GLU	B	287	13.621	-16.691	38.764	1.00	16.48	B
ATOM	5076	CG	GLU	B	287	15.094	-19.065	38.591	1.00	20.87	B
ATOM	5077	CD	GLU	B	287	15.613	-19.806	39.813	1.00	24.94	B
ATOM	5078	OE1	GLU	B	287	15.225	-20.975	40.008	1.00	28.92	B
ATOM	5079	OE2	GLU	B	287	16.400	-19.205	40.580	1.00	32.02	B
ATOM	5080	C	GLU	B	287	13.278	-18.314	36.296	1.00	15.72	B
ATOM	5081	O	GLU	B	287	12.644	-19.303	35.921	1.00	15.04	B
ATOM	5082	N	ASN	B	288	14.134	-17.655	35.518	1.00	14.89	B
ATOM	5083	CA	ASN	B	288	14.386	-18.021	34.127	1.00	15.81	B
ATOM	5084	CB	ASN	B	288	15.363	-19.200	34.049	1.00	17.29	B
ATOM	5085	CG	ASN	B	288	16.736	-18.812	34.607	1.00	19.00	B
ATOM	5086	OD1	ASN	B	288	17.095	-17.642	34.575	1.00	18.60	B
ATOM	5087	ND2	ASN	B	288	17.496	-19.779	35.122	1.00	22.68	B
ATOM	5088	C	ASN	B	288	13.146	-18.280	33.271	1.00	14.61	B
ATOM	5089	O	ASN	B	288	13.196	-19.064	32.325	1.00	15.72	B
ATOM	5090	N	GLN	B	289	12.047	-17.592	33.589	1.00	12.93	B
ATOM	5091	CA	GLN	B	289	10.834	-17.771	32.806	1.00	13.30	B
ATOM	5092	CB	GLN	B	289	9.979	-18.907	33.380	1.00	14.55	B
ATOM	5093	CG	GLN	B	289	8.664	-19.147	32.605	1.00	18.51	B
ATOM	5094	CD	GLN	B	289	7.737	-20.171	33.274	1.00	20.32	B
ATOM	5095	OE1	GLN	B	289	6.714	-19.820	33.912	1.00	24.66	B
ATOM	5096	NE2	GLN	B	289	8.084	-21.430	33.128	1.00	20.90	B
ATOM	5097	C	GLN	B	289	9.950	-16.543	32.706	1.00	13.31	B
ATOM	5098	O	GLN	B	289	9.796	-15.783	33.648	1.00	11.95	B
ATOM	5099	N	LEU	B	290	9.382	-16.347	31.513	1.00	12.64	B
ATOM	5100	CA	LEU	B	290	8.438	-15.253	31.315	1.00	13.02	B
ATOM	5101	CB	LEU	B	290	8.990	-14.220	30.294	1.00	14.05	B
ATOM	5102	CG	LEU	B	290	7.961	-13.160	29.861	1.00	15.71	B
ATOM	5103	CD1	LEU	B	290	7.482	-12.331	31.070	1.00	17.91	B
ATOM	5104	CD2	LEU	B	290	8.586	-12.240	28.816	1.00	17.17	B
ATOM	5105	C	LEU	B	290	7.155	-15.864	30.777	1.00	12.56	B
ATOM	5106	O	LEU	B	290	7.201	-16.657	29.836	1.00	14.23	B
ATOM	5107	N	LYS	B	291	6.022	-15.521	31.391	1.00	12.00	B
ATOM	5108	CA	LYS	B	291	4.723	-15.991	30.909	1.00	12.78	B
ATOM	5109	CB	LYS	B	291	3.958	-16.744	32.014	1.00	14.55	B
ATOM	5110	CG	LYS	B	291	2.521	-17.061	31.604	1.00	17.33	B
ATOM	5111	CD	LYS	B	291	1.794	-17.803	32.734	1.00	23.96	B
ATOM	5112	CE	LYS	B	291	0.313	-17.910	32.428	1.00	28.19	B
ATOM	5113	NZ	LYS	B	291	-0.532	-18.367	33.595	1.00	33.90	B
ATOM	5114	C	LYS	B	291	3.975	-14.725	30.480	1.00	13.62	B
ATOM	5115	O	LYS	B	291	3.869	-13.757	31.243	1.00	15.74	B
ATOM	5116	N	ILE	B	292	3.487	-14.708	29.241	1.00	11.68	B
ATOM	5117	CA	ILE	B	292	2.736	-13.572	28.712	1.00	12.10	B
ATOM	5118	CB	ILE	B	292	3.318	-13.132	27.329	1.00	12.34	B
ATOM	5119	CG2	ILE	B	292	2.448	-12.013	26.690	1.00	14.58	B
ATOM	5120	CG1	ILE	B	292	4.739	-12.646	27.525	1.00	15.22	B
ATOM	5121	CD1	ILE	B	292	5.529	-12.532	26.240	1.00	17.04	B
ATOM	5122	C	ILE	B	292	1.303	-14.048	28.511	1.00	12.60	B
ATOM	5123	O	ILE	B	292	1.075	-15.065	27.844	1.00	13.06	B
ATOM	5124	N	THR	B	293	0.340	-13.316	29.072	1.00	12.37	B
ATOM	5125	CA	THR	B	293	-1.050	-13.703	28.891	1.00	13.44	B
ATOM	5126	CB	THR	B	293	-1.699	-14.182	30.200	1.00	14.23	B
ATOM	5127	OG1	THR	B	293	-1.641	-13.160	31.179	1.00	18.90	B
ATOM	5128	CG2	THR	B	293	-0.947	-15.366	30.766	1.00	15.88	B
ATOM	5129	C	THR	B	293	-1.832	-12.525	28.372	1.00	14.34	B
ATOM	5130	O	THR	B	293	-1.471	-11.362	28.600	1.00	13.84	B
ATOM	5131	N	ALA	B	294	-2.883	-12.837	27.634	1.00	12.99	B
ATOM	5132	CA	ALA	B	294	-3.746	-11.800	27.101	1.00	14.01	B
ATOM	5133	CB	ALA	B	294	-3.325	-11.469	25.644	1.00	15.00	B
ATOM	5134	C	ALA	B	294	-5.164	-12.333	27.116	1.00	15.21	B
ATOM	5135	O	ALA	B	294	-5.383	-13.509	26.864	1.00	15.46	B
ATOM	5136	N	ASN	B	295	-6.132	-11.486	27.461	1.00	15.97	B
ATOM	5137	CA	ASN	B	295	-7.515	-11.907	27.367	1.00	17.95	B
ATOM	5138	CB	ASN	B	295	-8.052	-12.461	28.700	1.00	23.39	B
ATOM	5139	CG	ASN	B	295	-8.003	-11.480	29.817	1.00	25.82	B
ATOM	5140	OD1	ASN	B	295	-8.523	-10.373	29.718	1.00	31.67	B
ATOM	5141	ND2	ASN	B	295	-7.393	-11.888	30.929	1.00	32.50	B
ATOM	5142	C	ASN	B	295	-8.325	-10.718	26.865	1.00	16.88	B
ATOM	5143	O	ASN	B	295	-7.873	-9.568	26.935	1.00	17.31	B
ATOM	5144	N	ASN	B	296	-9.499	-10.996	26.302	1.00	16.35	B
ATOM	5145	CA	ASN	B	296	-10.311	-9.920	25.755	1.00	17.61	B
ATOM	5146	CB	ASN	B	296	-10.294	-9.966	24.205	1.00	16.78	B
ATOM	5147	CG	ASN	B	296	-10.835	-11.274	23.639	1.00	17.58	B
ATOM	5148	OD1	ASN	B	296	-11.629	-11.955	24.285	1.00	19.52	B
ATOM	5149	ND2	ASN	B	296	-10.438	-11.601	22.407	1.00	18.80	B
ATOM	5150	C	ASN	B	296	-11.734	-10.022	26.306	1.00	18.87	B
ATOM	5151	O	ASN	B	296	-12.049	-10.878	27.141	1.00	18.85	B
ATOM	5152	N	PRO	B	297	-12.603	-9.111	25.877	1.00	22.70	B
ATOM	5153	CD	PRO	B	297	-12.351	-7.873	25.120	1.00	23.09	B
ATOM	5154	CA	PRO	B	297	-13.975	-9.157	26.373	1.00	25.09	B
ATOM	5155	CB	PRO	B	297	-14.586	-7.858	25.842	1.00	25.02	B
ATOM	5156	CG	PRO	B	297	-13.432	-6.952	25.666	1.00	23.49	B
ATOM	5157	C	PRO	B	297	-14.773	-10.376	25.925	1.00	26.91	B
ATOM	5158	O	PRO	B	297	-15.828	-10.638	26.490	1.00	29.58	B
ATOM	5159	N	GLU	B	298	-14.317	-11.085	24.893	1.00	28.28	B
ATOM	5160	CA	GLU	B	298	-15.033	-12.275	24.425	1.00	29.32	B
ATOM	5161	CB	GLU	B	298	-14.805	-12.487	22.919	1.00	33.72	B
ATOM	5162	CG	GLU	B	298	-15.968	-12.033	22.025	1.00	38.43	B
ATOM	5163	CD	GLU	B	298	-16.282	-10.547	22.144	1.00	42.52	B
ATOM	5164	OE1	GLU	B	298	-15.362	-9.730	21.889	1.00	43.73	B
ATOM	5165	OE2	GLU	B	298	-17.449	-10.200	22.490	1.00	43.97	B

Figure 1 (continued 52)

ATOM	5166	C	GLU	B	298	-14.606	-13.524	25.205	1.00 28.60	B
ATOM	5167	O	GLU	B	298	-14.936	-14.643	24.817	1.00 27.81	B
ATOM	5168	N	GLN	B	299	-13.870	-13.325	26.301	1.00 27.28	B
ATOM	5169	CA	GLN	B	299	-13.431	-14.434	27.148	1.00 27.04	B
ATOM	5170	CB	GLN	B	299	-14.615	-15.356	27.468	1.00 30.88	B
ATOM	5171	CG	GLN	B	299	-15.432	-15.000	28.711	1.00 37.59	B
ATOM	5172	CD	GLN	B	299	-15.844	-13.553	28.768	1.00 40.60	B
ATOM	5173	OE1	GLN	B	299	-15.062	-12.682	29.185	1.00 42.63	B
ATOM	5174	NE2	GLN	B	299	-17.080	-13.273	28.344	1.00 42.73	B
ATOM	5175	C	GLN	B	299	-12.326	-15.273	26.516	1.00 22.97	B
ATOM	5176	O	GLN	B	299	-12.014	-16.375	26.995	1.00 21.99	B
ATOM	5177	N	GLU	B	300	-11.762	-14.769	25.428	1.00 19.48	B
ATOM	5178	CA	GLU	B	300	-10.680	-15.479	24.756	1.00 15.67	B
ATOM	5179	CB	GLU	B	300	-10.583	-15.026	23.291	1.00 15.71	B
ATOM	5180	CG	GLU	B	300	-11.879	-15.412	22.546	1.00 16.99	B
ATOM	5181	CD	GLU	B	300	-11.936	-14.867	21.148	1.00 17.62	B
ATOM	5182	OE1	GLU	B	300	-11.425	-13.753	20.908	1.00 19.18	B
ATOM	5183	OE2	GLU	B	300	-12.507	-15.566	20.289	1.00 18.81	B
ATOM	5184	C	GLU	B	300	-9.395	-15.245	25.501	1.00 17.24	B
ATOM	5185	O	GLU	B	300	-9.223	-14.200	26.160	1.00 15.99	B
ATOM	5186	N	GLU	B	301	-8.487	-16.212	25.407	1.00 15.46	B
ATOM	5187	CA	GLU	B	301	-7.239	-16.084	26.143	1.00 16.90	B
ATOM	5188	CB	GLU	B	301	-7.305	-16.893	27.436	1.00 21.09	B
ATOM	5189	CG	GLU	B	301	-8.146	-16.367	28.543	1.00 30.92	B
ATOM	5190	CD	GLU	B	301	-7.962	-17.237	29.766	1.00 35.02	B
ATOM	5191	OE1	GLU	B	301	-6.789	-17.389	30.212	1.00 38.01	B
ATOM	5192	OE2	GLU	B	301	-8.979	-17.773	30.255	1.00 38.32	B
ATOM	5193	C	GLU	B	301	-6.073	-16.632	25.401	1.00 15.82	B
ATOM	5194	O	GLU	B	301	-6.198	-17.658	24.748	1.00 15.36	B
ATOM	5195	N	ALA	B	302	-4.931	-15.953	25.537	1.00 14.54	B
ATOM	5196	CA	ALA	B	302	-3.688	-16.427	24.943	1.00 14.01	B
ATOM	5197	CB	ALA	B	302	-3.195	-15.479	23.876	1.00 15.13	B
ATOM	5198	C	ALA	B	302	-2.644	-16.540	26.060	1.00 14.66	B
ATOM	5199	O	ALA	B	302	-2.640	-15.741	27.006	1.00 16.02	B
ATOM	5200	N	GLU	B	303	-1.782	-17.553	25.969	1.00 13.72	B
ATOM	5201	CA	GLU	B	303	-0.691	-17.712	26.953	1.00 13.49	B
ATOM	5202	CB	GLU	B	303	-1.021	-18.772	28.011	1.00 14.66	B
ATOM	5203	CG	GLU	B	303	0.164	-19.059	28.960	1.00 18.75	B
ATOM	5204	CD	GLU	B	303	-0.155	-20.148	29.970	1.00 23.21	B
ATOM	5205	OE1	GLU	B	303	-0.967	-19.881	30.873	1.00 26.03	B
ATOM	5206	OE2	GLU	B	303	0.387	-21.261	29.853	1.00 23.17	B
ATOM	5207	C	GLU	B	303	0.559	-18.156	26.209	1.00 12.96	B
ATOM	5208	O	GLU	B	303	0.502	-19.062	25.366	1.00 12.70	B
ATOM	5209	N	GLU	B	304	1.667	-17.486	26.485	1.00 11.86	B
ATOM	5210	CA	GLU	B	304	2.955	-17.833	25.880	1.00 12.51	B
ATOM	5211	CB	GLU	B	304	3.474	-16.692	24.994	1.00 12.92	B
ATOM	5212	CG	GLU	B	304	2.613	-16.412	23.768	1.00 13.88	B
ATOM	5213	CD	GLU	B	304	2.846	-17.416	22.654	1.00 16.15	B
ATOM	5214	OE1	GLU	B	304	3.836	-18.173	22.717	1.00 14.88	B
ATOM	5215	OE2	GLU	B	304	2.029	-17.448	21.702	1.00 16.52	B
ATOM	5216	C	GLU	B	304	3.958	-18.009	27.014	1.00 12.92	B
ATOM	5217	O	GLU	B	304	4.033	-17.156	27.894	1.00 13.66	B
ATOM	5218	N	ILE	B	305	4.718	-19.108	27.010	1.00 12.77	B
ATOM	5219	CA	ILE	B	305	5.738	-19.283	28.037	1.00 11.99	B
ATOM	5220	CB	ILE	B	305	5.549	-20.605	28.791	1.00 13.43	B
ATOM	5221	CG2	ILE	B	305	6.730	-20.801	29.771	1.00 14.23	B
ATOM	5222	CG1	ILE	B	305	4.211	-20.536	29.555	1.00 15.50	B
ATOM	5223	CD1	ILE	B	305	3.773	-21.908	30.095	1.00 21.38	B
ATOM	5224	C	ILE	B	305	7.074	-19.263	27.309	1.00 13.39	B
ATOM	5225	O	ILE	B	305	7.206	-19.891	26.239	1.00 14.67	B
ATOM	5226	N	LEU	B	306	8.033	-18.501	27.838	1.00 12.78	B
ATOM	5227	CA	LEU	B	306	9.363	-18.388	27.201	1.00 13.06	B
ATOM	5228	CB	LEU	B	306	9.567	-16.973	26.621	1.00 16.49	B
ATOM	5229	CG	LEU	B	306	8.629	-16.459	25.530	1.00 19.31	B
ATOM	5230	CD1	LEU	B	306	8.803	-14.943	25.356	1.00 22.78	B
ATOM	5231	CD2	LEU	B	306	8.922	-17.216	24.223	1.00 21.99	B
ATOM	5232	C	LEU	B	306	10.473	-18.598	28.221	1.00 13.14	B
ATOM	5233	O	LEU	B	306	10.347	-18.191	29.368	1.00 13.66	B
ATOM	5234	N	ASP	B	307	11.579	-19.197	27.784	1.00 14.05	B
ATOM	5235	CA	ASP	B	307	12.724	-19.322	28.668	1.00 14.97	B
ATOM	5236	CB	ASP	B	307	13.664	-20.441	28.216	1.00 17.59	B
ATOM	5237	CG	ASP	B	307	13.064	-21.815	28.375	1.00 21.45	B
ATOM	5238	OD1	ASP	B	307	12.257	-22.018	29.283	1.00 21.70	B
ATOM	5239	OD2	ASP	B	307	13.415	-22.718	27.587	1.00 29.43	B
ATOM	5240	C	ASP	B	307	13.472	-17.998	28.538	1.00 16.22	B
ATOM	5241	O	ASP	B	307	13.683	-17.502	27.407	1.00 17.41	B
ATOM	5242	N	VAL	B	308	13.856	-17.419	29.672	1.00 15.42	B
ATOM	5243	CA	VAL	B	308	14.622	-16.170	29.691	1.00 16.59	B
ATOM	5244	CB	VAL	B	308	13.719	-14.932	29.974	1.00 16.08	B
ATOM	5245	CG1	VAL	B	308	12.596	-14.869	28.938	1.00 14.76	B
ATOM	5246	CG2	VAL	B	308	13.156	-14.972	31.412	1.00 15.53	B
ATOM	5247	C	VAL	B	308	15.661	-16.311	30.800	1.00 18.09	B
ATOM	5248	O	VAL	B	308	15.705	-17.332	31.479	1.00 18.24	B
ATOM	5249	N	THR	B	309	16.540	-15.320	30.928	1.00 17.26	B
ATOM	5250	CA	THR	B	309	17.514	-15.322	32.010	1.00 19.28	B
ATOM	5251	CB	THR	B	309	18.901	-14.815	31.545	1.00 19.61	B
ATOM	5252	OG1	THR	B	309	19.416	-15.679	30.540	1.00 21.13	B
ATOM	5253	CG2	THR	B	309	19.879	-14.794	32.712	1.00 23.93	B
ATOM	5254	C	THR	B	309	16.944	-14.334	33.032	1.00 18.30	B
ATOM	5255	O	THR	B	309	16.798	-13.147	32.747	1.00 20.11	B
ATOM	5256	N	TYR	B	310	16.577	-14.826	34.215	1.00 18.66	B
ATOM	5257	CA	TYR	B	310	16.037	-13.957	35.261	1.00 16.85	B
ATOM	5258	CB	TYR	B	310	14.537	-13.655	35.065	1.00 17.90	B
ATOM	5259	CG	TYR	B	310	13.993	-12.756	36.152	1.00 18.11	B
ATOM	5260	CD1	TYR	B	310	14.389	-11.420	36.234	1.00 19.98	B
ATOM	5261	CE1	TYR	B	310	13.958	-10.596	37.265	1.00 21.65	B
ATOM	5262	CD2	TYR	B	310	13.135	-13.241	37.142	1.00 18.77	B
ATOM	5263	CE2	TYR	B	310	12.694	-12.428	38.168	1.00 19.14	B
ATOM	5264	CZ	TYR	B	310	13.100	-11.111	38.239	1.00 22.59	B
ATOM	5265	OH	TYR	B	310	12.642	-10.325	39.276	1.00 23.29	B

Figure 1 (continued 53)

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ATOM   5266  C    TYR B 310    16.202 -14.605  36.635  1.00 20.33        B
ATOM   5267  O    TYR B 310    15.861 -15.775  36.802  1.00 18.99        B
ATOM   5268  N    SER B 311    16.711 -13.831  37.604  1.00 21.68        B
ATOM   5269  CA   SER B 311    16.890 -14.340  38.973  1.00 25.75        B
ATOM   5270  CB   SER B 311    18.376 -14.490  39.291  1.00 27.17        B
ATOM   5271  OG   SER B 311    18.819 -15.761  38.877  1.00 32.61        B
ATOM   5272  C    SER B 311    16.229 -13.539  40.094  1.00 27.05        B
ATOM   5273  O    SER B 311    16.370 -13.876  41.264  1.00 31.83        B
ATOM   5274  N    GLY B 312    15.500 -12.481  39.778  1.00 28.46        B
ATOM   5275  CA   GLY B 312    14.864 -11.724  40.848  1.00 28.43        B
ATOM   5276  C    GLY B 312    13.588 -12.299  41.478  1.00 27.94        B
ATOM   5277  O    GLY B 312    13.187 -13.451  41.239  1.00 26.97        B
ATOM   5278  N    ALA B 313    12.957 -11.478  42.210  1.00 26.88        B
ATOM   5279  CA   ALA B 313    11.711 -11.848  42.966  1.00 24.05        B
ATOM   5280  CB   ALA B 313    11.312 -10.763  43.966  1.00 24.56        B
ATOM   5281  C    ALA B 313    10.665 -11.932  41.853  1.00 22.56        B
ATOM   5282  O    ALA B 313    10.806 -11.298  40.799  1.00 20.08        B
ATOM   5283  N    GLU B 314     9.618 -12.725  42.066  1.00 19.40        B
ATOM   5284  CA   GLU B 314     8.586 -12.840  41.042  1.00 18.07        B
ATOM   5285  CB   GLU B 314     7.647 -14.039  41.323  1.00 16.92        B
ATOM   5286  CG   GLU B 314     8.410 -15.354  41.405  1.00 16.41        B
ATOM   5287  CD   GLU B 314     7.525 -16.589  41.365  1.00 14.40        B
ATOM   5288  OE1  GLU B 314     6.317 -16.485  41.643  1.00 15.57        B
ATOM   5289  OE2  GLU B 314     8.058 -17.668  41.064  1.00 17.05        B
ATOM   5290  C    GLU B 314     7.772 -11.565  41.032  1.00 17.69        B
ATOM   5291  O    GLU B 314     7.685 -10.870  42.033  1.00 18.99        B
ATOM   5292  N    MET B 315     7.209 -11.226  39.878  1.00 18.30        B
ATOM   5293  CA   MET B 315     6.352 -10.044  39.793  1.00 16.99        B
ATOM   5294  CB   MET B 315     7.156  -8.741  39.754  1.00 19.43        B
ATOM   5295  CG   MET B 315     8.052  -8.587  38.571  1.00 18.90        B
ATOM   5296  SD   MET B 315     8.654  -6.862  38.490  1.00 23.78        B
ATOM   5297  CE   MET B 315     7.247  -6.033  37.765  1.00 21.20        B
ATOM   5298  C    MET B 315     5.509 -10.144  38.542  1.00 18.24        B
ATOM   5299  O    MET B 315     5.833 -10.890  37.618  1.00 16.64        B
ATOM   5300  N    GLU B 316     4.404  -9.423  38.554  1.00 17.91        B
ATOM   5301  CA   GLU B 316     3.499  -9.387  37.442  1.00 19.14        B
ATOM   5302  CB   GLU B 316     2.153  -9.964  37.876  1.00 22.45        B
ATOM   5303  CG   GLU B 316     1.183 -10.293  36.755  1.00 30.42        B
ATOM   5304  CD   GLU B 316    -0.058 -11.022  37.282  1.00 33.19        B
ATOM   5305  OE1  GLU B 316    -0.126 -12.269  37.189  1.00 36.29        B
ATOM   5306  OE2  GLU B 316    -0.957 -10.337  37.807  1.00 35.89        B
ATOM   5307  C    GLU B 316     3.374  -7.916  37.058  1.00 18.61        B
ATOM   5308  O    GLU B 316     3.442  -7.029  37.917  1.00 19.48        B
ATOM   5309  N    ILE B 317     3.202  -7.651  35.770  1.00 17.17        B
ATOM   5310  CA   ILE B 317     3.090  -6.281  35.317  1.00 14.40        B
ATOM   5311  CB   ILE B 317     4.500  -5.648  35.163  1.00 14.99        B
ATOM   5312  CG2  ILE B 317     5.382  -6.449  34.166  1.00 15.39        B
ATOM   5313  CG1  ILE B 317     4.373  -4.195  34.724  1.00 16.07        B
ATOM   5314  CD1  ILE B 317     5.731  -3.450  34.830  1.00 16.39        B
ATOM   5315  C    ILE B 317     2.319  -6.249  34.003  1.00 15.91        B
ATOM   5316  O    ILE B 317     2.484  -7.144  33.166  1.00 15.36        B
ATOM   5317  N    GLY B 318     1.489  -5.225  33.826  1.00 15.37        B
ATOM   5318  CA   GLY B 318     0.701  -5.121  32.611  1.00 13.91        B
ATOM   5319  C    GLY B 318     1.261  -4.061  31.670  1.00 15.48        B
ATOM   5320  O    GLY B 318     1.888  -3.115  32.135  1.00 14.18        B
ATOM   5321  N    PHE B 319     1.072  -4.255  30.363  1.00 15.89        B
ATOM   5322  CA   PHE B 319     1.513  -3.311  29.331  1.00 16.03        B
ATOM   5323  CB   PHE B 319     2.897  -3.692  28.777  1.00 17.13        B
ATOM   5324  CG   PHE B 319     4.022  -3.383  29.686  1.00 18.79        B
ATOM   5325  CD1  PHE B 319     4.434  -2.073  29.877  1.00 21.89        B
ATOM   5326  CD2  PHE B 319     4.673  -4.401  30.368  1.00 21.55        B
ATOM   5327  CE1  PHE B 319     5.481  -1.786  30.740  1.00 22.47        B
ATOM   5328  CE2  PHE B 319     5.716  -4.122  31.236  1.00 21.80        B
ATOM   5329  CZ   PHE B 319     6.121  -2.820  31.423  1.00 23.74        B
ATOM   5330  C    PHE B 319     0.602  -3.282  28.129  1.00 16.79        B
ATOM   5331  O    PHE B 319    -0.122  -4.242  27.846  1.00 16.37        B
ATOM   5332  N    ASN B 320     0.635  -2.143  27.431  1.00 16.27        B
ATOM   5333  CA   ASN B 320    -0.051  -1.983  26.158  1.00 16.46        B
ATOM   5334  CB   ASN B 320    -0.055  -0.504  25.796  1.00 18.69       \B
ATOM   5335  CG   ASN B 320    -0.561  -0.259  24.407  1.00 18.32       \B
ATOM   5336  OD1  ASN B 320    -0.226  -0.997  23.481  1.00 18.44        B
ATOM   5337  ND2  ASN B 320    -1.362   0.791  24.242  1.00 18.81        B
ATOM   5338  C    ASN B 320     0.927  -2.745  25.249  1.00 17.08        B
ATOM   5339  O    ASN B 320     2.093  -2.350  25.102  1.00 16.27        B
ATOM   5340  N    VAL B 321     0.478  -3.843  24.645  1.00 15.94        B
ATOM   5341  CA   VAL B 321     1.379  -4.662  23.845  1.00 16.35        B
ATOM   5342  CB   VAL B 321     0.703  -6.027  23.464  1.00 16.49        B
ATOM   5343  CG1  VAL B 321    -0.409  -5.817  22.450  1.00 17.69        B
ATOM   5344  CG2  VAL B 321     1.743  -7.004  22.956  1.00 14.64        B
ATOM   5345  C    VAL B 321     1.891  -3.939  22.610  1.00 17.10        B
ATOM   5346  O    VAL B 321     2.977  -4.245  22.119  1.00 15.35        B
ATOM   5347  N    SER B 322     1.146  -2.961  22.109  1.00 16.12        B
ATOM   5348  CA   SER B 322     1.657  -2.257  20.925  1.00 17.12        B
ATOM   5349  CB   SER B 322     0.587  -1.352  20.311  1.00 18.39        B
ATOM   5350  OG   SER B 322    -0.513  -2.129  19.863  1.00 22.65        B
ATOM   5351  C    SER B 322     2.899  -1.436  21.276  1.00 15.98        B
ATOM   5352  O    SER B 322     3.837  -1.353  20.468  1.00 15.16        B
ATOM   5353  N    TYR B 323     2.932  -0.853  22.482  1.00 14.24        B
ATOM   5354  CA   TYR B 323     4.110  -0.088  22.908  1.00 15.80        B
ATOM   5355  CB   TYR B 323     3.878   0.590  24.259  1.00 15.47        B
ATOM   5356  CG   TYR B 323     2.813   1.668  24.294  1.00 16.25        B
ATOM   5357  CD1  TYR B 323     2.397   2.314  23.127  1.00 19.59        B
ATOM   5358  CE1  TYR B 323     1.458   3.374  23.170  1.00 20.04        B
ATOM   5359  CD2  TYR B 323     2.284   2.093  25.509  1.00 18.22        B
ATOM   5360  CE2  TYR B 323     1.354   3.166  25.567  1.00 19.75        B
ATOM   5361  CZ   TYR B 323     0.957   3.790  24.399  1.00 21.19        B
ATOM   5362  OH   TYR B 323     0.112   4.886  24.453  1.00 23.64        B
ATOM   5363  C    TYR B 323     5.327  -1.018  23.041  1.00 15.80        B
ATOM   5364  O    TYR B 323     6.468  -0.646  22.726  1.00 15.87        B
ATOM   5365  N    VAL B 324     5.101  -2.226  23.563  1.00 14.85        B
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Figure 1 (continued 54)

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ATOM   5366  CA   VAL B 324      6.193   -3.182  23.687  1.00 14.69        B
ATOM   5367  CB   VAL B 324      5.776   -4.387  24.550  1.00 14.90        B
ATOM   5368  CG1  VAL B 324      6.913   -5.422  24.610  1.00 16.80        B
ATOM   5369  CG2  VAL B 324      5.440   -3.896  25.952  1.00 16.82        B
ATOM   5370  C    VAL B 324      6.674   -3.670  22.301  1.00 13.75        B
ATOM   5371  O    VAL B 324      7.885   -3.761  22.039  1.00 14.44        B
ATOM   5372  N    LEU B 325      5.737   -3.984  21.410  1.00 14.44        B
ATOM   5373  CA   LEU B 325      6.105   -4.424  20.085  1.00 13.52        B
ATOM   5374  CB   LEU B 325      4.852   -4.870  19.317  1.00 14.38        B
ATOM   5375  CG   LEU B 325      4.339   -6.244  19.774  1.00 14.30        B
ATOM   5376  CD1  LEU B 325      2.953   -6.506  19.170  1.00 15.19        B
ATOM   5377  CD2  LEU B 325      5.338   -7.346  19.363  1.00 14.63        B
ATOM   5378  C    LEU B 325      6.848   -3.319  19.334  1.00 14.06        B
ATOM   5379  O    LEU B 325      7.801   -3.603  18.606  1.00 15.63        B
ATOM   5380  N    ASP B 326      6.420   -2.074  19.503  1.00 14.14        B
ATOM   5381  CA   ASP B 326      7.113   -0.960  18.843  1.00 14.45        B
ATOM   5382  CB   ASP B 326      6.505    0.385  19.217  1.00 15.89        B
ATOM   5383  CG   ASP B 326      5.168    0.634  18.556  1.00 16.26        B
ATOM   5384  OD1  ASP B 326      4.803   -0.036  17.556  1.00 17.26        B
ATOM   5385  OD2  ASP B 326      4.471    1.551  19.018  1.00 18.69        B
ATOM   5386  C    ASP B 326      8.588   -0.952  19.255  1.00 14.86        B
ATOM   5387  O    ASP B 326      9.454   -0.768  18.416  1.00 15.93        B
ATOM   5388  N    VAL B 327      8.871   -1.163  20.542  1.00 15.32        B
ATOM   5389  CA   VAL B 327     10.246   -1.175  20.989  1.00 15.55        B
ATOM   5390  CB   VAL B 327     10.301   -1.226  22.534  1.00 16.32        B
ATOM   5391  CG1  VAL B 327     11.715   -1.474  22.996  1.00 15.81        B
ATOM   5392  CG2  VAL B 327      9.783    0.086  23.085  1.00 15.65        B
ATOM   5393  C    VAL B 327     11.039   -2.352  20.422  1.00 16.20        B
ATOM   5394  O    VAL B 327     12.179   -2.184  19.974  1.00 15.94        B
ATOM   5395  N    LEU B 328     10.437   -3.547  20.435  1.00 14.84        B
ATOM   5396  CA   LEU B 328     11.150   -4.726  19.961  1.00 15.54        B
ATOM   5397  CB   LEU B 328     10.347   -5.985  20.295  1.00 14.62        B
ATOM   5398  CG   LEU B 328     10.130   -6.193  21.808  1.00 15.10        B
ATOM   5399  CD1  LEU B 328      9.295   -7.460  22.024  1.00 14.68        B
ATOM   5400  CD2  LEU B 328     11.503   -6.337  22.497  1.00 16.58        B
ATOM   5401  C    LEU B 328     11.416   -4.600  18.480  1.00 16.34        B
ATOM   5402  O    LEU B 328     12.455   -5.042  17.998  1.00 17.56        B
ATOM   5403  N    ASN B 329     10.491   -3.970  17.758  1.00 17.06        B
ATOM   5404  CA   ASN B 329     10.680   -3.755  16.332  1.00 20.23        B
ATOM   5405  CB   ASN B 329      9.371   -3.285  15.675  1.00 20.68        B
ATOM   5406  CG   ASN B 329      8.414   -4.440  15.381  1.00 25.15        B
ATOM   5407  OD1  ASN B 329      7.193   -4.308  15.536  1.00 29.33        B
ATOM   5408  ND2  ASN B 329      8.961   -5.571  14.932  1.00 25.44        B
ATOM   5409  C    ASN B 329     11.790   -2.743  16.076  1.00 20.26        B
ATOM   5410  O    ASN B 329     12.504   -2.875  15.074  1.00 21.57        B
ATOM   5411  N    ALA B 330     11.958   -1.754  16.963  1.00 19.54        B
ATOM   5412  CA   ALA B 330     13.007   -0.741  16.795  1.00 20.36        B
ATOM   5413  CB   ALA B 330     12.703    0.488  17.630  1.00 19.00        B
ATOM   5414  C    ALA B 330     14.392   -1.275  17.151  1.00 22.18        B
ATOM   5415  O    ALA B 330     15.410   -0.786  16.652  1.00 22.02        B
ATOM   5416  N    LEU B 331     14.425   -2.269  18.031  1.00 22.79        B
ATOM   5417  CA   LEU B 331     15.675   -2.900  18.445  1.00 26.40        B
ATOM   5418  CB   LEU B 331     15.542   -3.459  19.876  1.00 24.34        B
ATOM   5419  CG   LEU B 331     15.521   -2.496  21.077  1.00 23.11        B
ATOM   5420  CD1  LEU B 331     15.059   -3.251  22.320  1.00 23.07        B
ATOM   5421  CD2  LEU B 331     16.904   -1.904  21.324  1.00 22.88        B
ATOM   5422  C    LEU B 331     15.953   -4.042  17.466  1.00 29.87        B
ATOM   5423  O    LEU B 331     15.346   -5.118  17.543  1.00 32.92        B
ATOM   5424  N    LYS B 332     16.871   -3.831  16.540  1.00 32.35        B
ATOM   5425  CA   LYS B 332     17.157   -4.892  15.576  1.00 34.77        B
ATOM   5426  CB   LYS B 332     17.447   -4.281  14.205  1.00 37.40        B
ATOM   5427  CG   LYS B 332     18.504   -3.195  14.249  1.00 41.60        B
ATOM   5428  CD   LYS B 332     18.968   -2.812  12.865  1.00 44.04        B
ATOM   5429  CE   LYS B 332     20.404   -2.327  12.925  1.00 46.03        B
ATOM   5430  NZ   LYS B 332     21.304   -3.408  13.449  1.00 46.84        B
ATOM   5431  C    LYS B 332     18.364   -5.647  16.110  1.00 34.26        B
ATOM   5432  O    LYS B 332     19.478   -5.520  15.583  1.00 36.38        B
ATOM   5433  N    CYS B 333     18.139   -6.428  17.167  1.00 31.45        B
ATOM   5434  CA   CYS B 333     19.227   -7.147  17.809  1.00 28.74        B
ATOM   5435  CB   CYS B 333     19.682   -6.364  19.040  1.00 26.65        B
ATOM   5436  SG   CYS B 333     18.382   -6.128  20.301  1.00 24.29        B
ATOM   5437  C    CYS B 333     18.900   -8.582  18.201  1.00 27.77        B
ATOM   5438  O    CYS B 333     17.771   -9.039  18.057  1.00 27.74        B
ATOM   5439  N    GLU B 334     19.891   -9.292  18.722  1.00 24.94        B
ATOM   5440  CA   GLU B 334     19.651  -10.671  19.072  1.00 25.13        B
ATOM   5441  CB   GLU B 334     20.940  -11.490  19.059  1.00 28.75        B
ATOM   5442  CG   GLU B 334     20.639  -12.973  18.832  1.00 33.58        B
ATOM   5443  CD   GLU B 334     21.798  -13.903  19.171  1.00 37.85        B
ATOM   5444  OE1  GLU B 334     22.835  -13.880  18.469  1.00 38.76        B
ATOM   5445  OE2  GLU B 334     21.656  -14.670  20.151  1.00 39.90        B
ATOM   5446  C    GLU B 334     18.977  -10.831  20.420  1.00 22.72        B
ATOM   5447  O    GLU B 334     18.060  -11.628  20.559  1.00 22.05        B
ATOM   5448  N    ASN B 335     19.449  -10.089  21.410  1.00 21.54        B
ATOM   5449  CA   ASN B 335     18.873  -10.202  22.751  1.00 21.37        B
ATOM   5450  CB   ASN B 335     19.841  -10.945  23.673  1.00 22.21        B
ATOM   5451  CG   ASN B 335     20.230  -12.327  23.127  1.00 23.10        B
ATOM   5452  OD1  ASN B 335     21.320  -12.515  22.569  1.00 27.23        B
ATOM   5453  ND2  ASN B 335     19.349  -13.283  23.283  1.00 20.66        B
ATOM   5454  C    ASN B 335     18.540   -8.849  23.347  1.00 21.05        B
ATOM   5455  O    ASN B 335     19.193   -7.848  23.057  1.00 19.95        B
ATOM   5456  N    VAL B 336     17.499   -8.824  24.174  1.00 18.30        B
ATOM   5457  CA   VAL B 336     17.074   -7.600  24.817  1.00 18.62        B
ATOM   5458  CB   VAL B 336     15.629   -7.224  24.418  1.00 19.11        B
ATOM   5459  CG1  VAL B 336     15.564   -6.941  22.908  1.00 19.33        B
ATOM   5460  CG2  VAL B 336     14.681   -8.367  24.762  1.00 23.69        B
ATOM   5461  C    VAL B 336     17.118   -7.770  26.331  1.00 19.78        B
ATOM   5462  O    VAL B 336     17.054   -8.896  26.846  1.00 20.30        B
ATOM   5463  N    ARG B 337     17.243   -6.644  27.022  1.00 18.96        B
ATOM   5464  CA   ARG B 337     17.259   -6.617  28.482  1.00 19.16        B
ATOM   5465  CB   ARG B 337     18.589   -6.071  29.016  1.00 20.68        B
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Figure 1 (continued 55)

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ATOM   5466  CG   ARG B 337      18.600   -5.938   30.554  1.00 23.91      B
ATOM   5467  CD   ARG B 337      19.995   -5.583   31.102  1.00 23.98      B
ATOM   5468  NE   ARG B 337      21.011   -6.545   30.668  1.00 27.10      B
ATOM   5469  CZ   ARG B 337      21.895   -6.313   29.704  1.00 26.89      B
ATOM   5470  NH1  ARG B 337      21.898   -5.149   29.068  1.00 28.48      B
ATOM   5471  NH2  ARG B 337      22.773   -7.244   29.371  1.00 28.51      B
ATOM   5472  C    ARG B 337      16.134   -5.715   28.938  1.00 19.09      B
ATOM   5473  O    ARG B 337      15.996   -4.586   28.465  1.00 18.29      B
ATOM   5474  N    MET B 338      15.293   -6.223   29.835  1.00 18.31      B
ATOM   5475  CA   MET B 338      14.197   -5.456   30.392  1.00 19.62      B
ATOM   5476  CB   MET B 338      12.884   -6.241   30.331  1.00 20.28      B
ATOM   5477  CG   MET B 338      12.410   -6.552   28.924  1.00 23.02      B
ATOM   5478  SD   MET B 338      10.698   -7.188   28.918  1.00 30.58      B
ATOM   5479  CE   MET B 338      10.105   -6.371   30.539  1.00 23.41      B
ATOM   5480  C    MET B 338      14.585   -5.245   31.843  1.00 19.01      B
ATOM   5481  O    MET B 338      14.968   -6.203   32.527  1.00 19.47      B
ATOM   5482  N    MET B 339      14.491   -4.008   32.302  1.00 20.01      B
ATOM   5483  CA   MET B 339      14.840   -3.658   33.682  1.00 19.93      B
ATOM   5484  CB   MET B 339      15.951   -2.600   33.651  1.00 23.82      B
ATOM   5485  CG   MET B 339      17.044   -3.049   32.682  1.00 28.37      B
ATOM   5486  SD   MET B 339      18.055   -1.714   32.046  1.00 39.00      B
ATOM   5487  CE   MET B 339      19.307   -1.887   33.240  1.00 33.07      B
ATOM   5488  C    MET B 339      13.570   -3.191   34.385  1.00 18.83      B
ATOM   5489  O    MET B 339      12.958   -2.204   34.009  1.00 16.91      B
ATOM   5490  N    LEU B 340      13.174   -3.940   35.420  1.00 18.32      B
ATOM   5491  CA   LEU B 340      11.927   -3.673   36.114  1.00 20.68      B
ATOM   5492  CB   LEU B 340      11.036   -4.916   36.055  1.00 23.79      B
ATOM   5493  CG   LEU B 340      10.657   -5.377   34.649  1.00 25.40      B
ATOM   5494  CD1  LEU B 340      11.509   -6.576   34.276  1.00 29.66      B
ATOM   5495  CD2  LEU B 340       9.190   -5.735   34.630  1.00 28.50      B
ATOM   5496  C    LEU B 340      12.104   -3.309   37.555  1.00 19.92      B
ATOM   5497  O    LEU B 340      13.150   -3.553   38.135  1.00 21.79      B
ATOM   5498  N    THR B 341      11.055   -2.720   38.116  1.00 23.10      B
ATOM   5499  CA   THR B 341      11.045   -2.310   39.509  1.00 25.27      B
ATOM   5500  CB   THR B 341      10.910   -0.789   39.596  1.00 26.79      B
ATOM   5501  OG1  THR B 341      12.026   -0.190   38.911  1.00 28.07      B
ATOM   5502  CG2  THR B 341      10.904   -0.337   41.053  1.00 26.69      B
ATOM   5503  C    THR B 341       9.863   -3.015   40.164  1.00 25.85      B
ATOM   5504  O    THR B 341      10.041   -3.872   41.028  1.00 28.86      B
ATOM   5505  N    ASP B 342       8.653   -2.670   39.735  1.00 25.54      B
ATOM   5506  CA   ASP B 342       7.466   -3.300   40.266  1.00 25.04      B
ATOM   5507  CB   ASP B 342       7.138   -2.742   41.651  1.00 25.70      B
ATOM   5508  CG   ASP B 342       6.999   -1.236   41.650  1.00 27.01      B
ATOM   5509  OD1  ASP B 342       6.409   -0.692   40.701  1.00 23.85      B
ATOM   5510  OD2  ASP B 342       7.474   -0.587   42.615  1.00 29.24      B
ATOM   5511  C    ASP B 342       6.309   -3.091   39.312  1.00 26.03      B
ATOM   5512  O    ASP B 342       6.469   -2.510   38.235  1.00 23.30      B
ATOM   5513  N    SER B 343       5.140   -3.581   39.700  1.00 24.63      B
ATOM   5514  CA   SER B 343       3.954   -3.490   38.866  1.00 26.73      B
ATOM   5515  CB   SER B 343       2.814   -4.253   39.519  1.00 27.90      B
ATOM   5516  OG   SER B 343       3.278   -5.495   39.991  1.00 33.35      B
ATOM   5517  C    SER B 343       3.445   -2.107   38.522  1.00 25.46      B
ATOM   5518  O    SER B 343       2.683   -1.947   37.568  1.00 27.08      B
ATOM   5519  N    VAL B 344       3.837   -1.100   39.291  1.00 25.08      B
ATOM   5520  CA   VAL B 344       3.324    0.227   39.030  1.00 23.51      B
ATOM   5521  CB   VAL B 344       2.676    0.818   40.318  1.00 24.60      B
ATOM   5522  CG1  VAL B 344       1.474   -0.026   40.725  1.00 27.19      B
ATOM   5523  CG2  VAL B 344       3.687    0.847   41.456  1.00 24.67      B
ATOM   5524  C    VAL B 344       4.405    1.163   38.512  1.00 23.49      B
ATOM   5525  O    VAL B 344       4.199    2.365   38.405  1.00 23.89      B
ATOM   5526  N    SER B 345       5.550    0.607   38.151  1.00 21.31      B
ATOM   5527  CA   SER B 345       6.617    1.467   37.691  1.00 20.87      B
ATOM   5528  CB   SER B 345       7.810    1.318   38.627  1.00 23.30      B
ATOM   5529  OG   SER B 345       7.409    1.696   39.946  1.00 21.45      B
ATOM   5530  C    SER B 345       7.012    1.166   36.260  1.00 21.79      B
ATOM   5531  O    SER B 345       6.770    0.077   35.761  1.00 21.63      B
ATOM   5532  N    SER B 346       7.618    2.153   35.615  1.00 21.53      B
ATOM   5533  CA   SER B 346       8.060    2.002   34.239  1.00 21.50      B
ATOM   5534  CB   SER B 346       8.655    3.320   33.722  1.00 21.47      B
ATOM   5535  OG   SER B 346       9.793    3.703   34.474  1.00 26.08      B
ATOM   5536  C    SER B 346       9.107    0.914   34.106  1.00 20.70      B
ATOM   5537  O    SER B 346       9.755    0.521   35.078  1.00 21.55      B
ATOM   5538  N    VAL B 347       9.255    0.411   32.890  1.00 21.06      B
ATOM   5539  CA   VAL B 347      10.254   -0.589   32.610  1.00 19.47      B
ATOM   5540  CB   VAL B 347       9.667   -1.886   31.960  1.00 21.64      B
ATOM   5541  CG1  VAL B 347       9.016   -1.578   30.636  1.00 22.58      B
ATOM   5542  CG2  VAL B 347      10.767   -2.905   31.746  1.00 22.90      B
ATOM   5543  C    VAL B 347      11.171    0.054   31.582  1.00 19.98      B
ATOM   5544  O    VAL B 347      10.705    0.845   30.758  1.00 19.77      B
ATOM   5545  N    GLN B 348      12.447   -0.270   31.667  1.00 18.29      B
ATOM   5546  CA   GLN B 348      13.421    0.211   30.694  1.00 19.12      B
ATOM   5547  CB   GLN B 348      14.667    0.811   31.375  1.00 21.07      B
ATOM   5548  CG   GLN B 348      15.791    1.231   30.385  1.00 24.52      B
ATOM   5549  CD   GLN B 348      16.826    2.140   31.039  1.00 25.62      B
ATOM   5550  OE1  GLN B 348      18.017    2.109   30.692  1.00 29.04      B
ATOM   5551  NE2  GLN B 348      16.378    2.944   31.980  1.00 25.26      B
ATOM   5552  C    GLN B 348      13.827   -0.987   29.863  1.00 18.81      B
ATOM   5553  O    GLN B 348      14.128   -2.070   30.398  1.00 19.57      B
ATOM   5554  N    ILE B 349      13.828   -0.811   28.539  1.00 16.48      B
ATOM   5555  CA   ILE B 349      14.216   -1.893   27.640  1.00 16.69      B
ATOM   5556  CB   ILE B 349      13.043   -2.317   26.739  1.00 15.20      B
ATOM   5557  CG2  ILE B 349      13.450   -3.542   25.886  1.00 15.51      B
ATOM   5558  CG1  ILE B 349      11.814   -2.594   27.628  1.00 14.39      B
ATOM   5559  CD1  ILE B 349      10.543   -2.916   26.841  1.00 16.74      B
ATOM   5560  C    ILE B 349      15.354   -1.434   26.757  1.00 16.84      B
ATOM   5561  O    ILE B 349      15.342   -0.309   26.258  1.00 17.09      B
ATOM   5562  N    GLU B 350      16.316   -2.315   26.555  1.00 18.33      B
ATOM   5563  CA   GLU B 350      17.477   -2.012   25.717  1.00 20.07      B
ATOM   5564  CB   GLU B 350      18.606   -1.403   26.573  1.00 22.27      B
ATOM   5565  CG   GLU B 350      18.629   -1.904   28.009  1.00 27.54      B
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Figure 1 (continued 56)

ATOM	5566	CD	GLU B 350	19.768	-1.317	28.861	1.00	28.87	B
ATOM	5567	OE1	GLU B 350	19.985	-0.085	28.838	1.00	30.71	B
ATOM	5568	OE2	GLU B 350	20.435	-2.111	29.569	1.00	32.23	B
ATOM	5569	C	GLU B 350	18.018	-3.247	25.033	1.00	20.43	B
ATOM	5570	O	GLU B 350	17.663	-4.385	25.373	1.00	19.39	B
ATOM	5571	N	ASP B 351	18.864	-3.023	24.030	1.00	18.78	B
ATOM	5572	CA	ASP B 351	19.556	-4.127	23.383	1.00	20.40	B
ATOM	5573	CB	ASP B 351	20.393	-3.559	22.216	1.00	20.92	B
ATOM	5574	CG	ASP B 351	21.276	-4.593	21.540	1.00	24.22	B
ATOM	5575	OD1	ASP B 351	21.520	-5.668	22.122	1.00	23.24	B
ATOM	5576	OD2	ASP B 351	21.747	-4.326	20.399	1.00	24.36	B
ATOM	5577	C	ASP B 351	20.480	-4.641	24.519	1.00	20.22	B
ATOM	5578	O	ASP B 351	21.154	-3.837	25.166	1.00	19.94	B
ATOM	5579	N	ALA B 352	20.513	-5.955	24.767	1.00	20.14	B
ATOM	5580	CA	ALA B 352	21.371	-6.512	25.828	1.00	22.88	B
ATOM	5581	CB	ALA B 352	21.102	-8.023	25.989	1.00	23.61	B
ATOM	5582	C	ALA B 352	22.856	-6.282	25.541	1.00	25.05	B
ATOM	5583	O	ALA B 352	23.687	-6.298	26.459	1.00	25.32	B
ATOM	5584	N	ALA B 353	23.187	-6.059	24.272	1.00	25.32	B
ATOM	5585	CA	ALA B 353	24.583	-5.871	23.874	1.00	27.92	B
ATOM	5586	CB	ALA B 353	24.888	-6.727	22.622	1.00	28.12	B
ATOM	5587	C	ALA B 353	25.008	-4.429	23.628	1.00	29.48	B
ATOM	5588	O	ALA B 353	26.134	-4.185	23.189	1.00	30.65	B
ATOM	5589	N	SER B 354	24.130	-3.471	23.895	1.00	28.82	B
ATOM	5590	CA	SER B 354	24.491	-2.068	23.695	1.00	30.09	B
ATOM	5591	CB	SER B 354	24.439	-1.695	22.213	1.00	30.87	B
ATOM	5592	OG	SER B 354	24.378	-0.282	22.073	1.00	30.83	B
ATOM	5593	C	SER B 354	23.612	-1.097	24.458	1.00	29.65	B
ATOM	5594	O	SER B 354	22.382	-1.233	24.488	1.00	29.50	B
ATOM	5595	N	GLN B 355	24.236	-0.096	25.064	1.00	29.47	B
ATOM	5596	CA	GLN B 355	23.475	0.900	25.794	1.00	29.78	B
ATOM	5597	CB	GLN B 355	24.227	1.337	27.057	1.00	33.08	B
ATOM	5598	CG	GLN B 355	24.449	0.245	28.091	1.00	37.90	B
ATOM	5599	CD	GLN B 355	25.421	0.691	29.180	1.00	41.35	B
ATOM	5600	OE1	GLN B 355	26.640	0.756	28.959	1.00	42.13	B
ATOM	5601	NE2	GLN B 355	24.883	1.026	30.355	1.00	42.11	B
ATOM	5602	C	GLN B 355	23.230	2.117	24.896	1.00	29.04	B
ATOM	5603	O	GLN B 355	22.833	3.167	25.389	1.00	29.11	B
ATOM	5604	N	SER B 356	23.439	1.963	23.586	1.00	28.20	B
ATOM	5605	CA	SER B 356	23.247	3.072	22.630	1.00	28.53	B
ATOM	5606	CB	SER B 356	23.499	2.600	21.187	1.00	29.22	B
ATOM	5607	OG	SER B 356	24.878	2.462	20.908	1.00	33.92	B
ATOM	5608	C	SER B 356	21.839	3.659	22.699	1.00	26.91	B
ATOM	5609	O	SER B 356	21.636	4.883	22.644	1.00	26.04	B
ATOM	5610	N	ALA B 357	20.849	2.782	22.801	1.00	24.78	B
ATOM	5611	CA	ALA B 357	19.476	3.240	22.852	1.00	23.09	B
ATOM	5612	CB	ALA B 357	18.707	2.773	21.599	1.00	23.03	B
ATOM	5613	C	ALA B 357	18.795	2.702	24.099	1.00	23.24	B
ATOM	5614	O	ALA B 357	19.167	1.646	24.625	1.00	25.22	B
ATOM	5615	N	ALA B 358	17.825	3.457	24.587	1.00	21.13	B
ATOM	5616	CA	ALA B 358	17.055	3.030	25.747	1.00	21.52	B
ATOM	5617	CB	ALA B 358	17.643	3.649	27.031	1.00	22.50	B
ATOM	5618	C	ALA B 358	15.585	3.402	25.566	1.00	19.54	B
ATOM	5619	O	ALA B 358	15.257	4.451	25.037	1.00	18.37	B
ATOM	5620	N	TYR B 359	14.683	2.527	26.017	1.00	18.21	B
ATOM	5621	CA	TYR B 359	13.259	2.747	25.886	1.00	18.06	B
ATOM	5622	CB	TYR B 359	12.642	1.724	24.919	1.00	17.72	B
ATOM	5623	CG	TYR B 359	13.303	1.776	23.558	1.00	15.03	B
ATOM	5624	CD1	TYR B 359	14.473	1.076	23.300	1.00	16.16	B
ATOM	5625	CE1	TYR B 359	15.151	1.242	22.104	1.00	14.13	B
ATOM	5626	CD2	TYR B 359	12.812	2.648	22.573	1.00	15.69	B
ATOM	5627	CE2	TYR B 359	13.485	2.819	21.379	1.00	13.85	B
ATOM	5628	CZ	TYR B 359	14.633	2.127	21.145	1.00	15.70	B
ATOM	5629	OH	TYR B 359	15.265	2.315	19.935	1.00	16.11	B
ATOM	5630	C	TYR B 359	12.597	2.609	27.235	1.00	19.04	B
ATOM	5631	O	TYR B 359	12.908	1.686	27.992	1.00	19.57	B
ATOM	5632	N	VAL B 360	11.730	3.546	27.545	1.00	17.94	B
ATOM	5633	CA	VAL B 360	11.023	3.501	28.812	1.00	19.18	B
ATOM	5634	CB	VAL B 360	11.276	4.794	29.641	1.00	18.75	B
ATOM	5635	CG1	VAL B 360	10.448	4.742	30.934	1.00	20.25	B
ATOM	5636	CG2	VAL B 360	12.753	4.923	29.937	1.00	19.41	B
ATOM	5637	C	VAL B 360	9.562	3.381	28.501	1.00	19.10	B
ATOM	5638	O	VAL B 360	9.008	4.188	27.753	1.00	19.90	B
ATOM	5639	N	VAL B 361	8.905	2.372	29.069	1.00	19.72	B
ATOM	5640	CA	VAL B 361	7.488	2.188	28.831	1.00	18.92	B
ATOM	5641	CB	VAL B 361	7.216	0.872	28.069	1.00	18.99	B
ATOM	5642	CG1	VAL B 361	5.743	0.769	27.716	1.00	18.31	B
ATOM	5643	CG2	VAL B 361	8.065	0.839	26.786	1.00	17.76	B
ATOM	5644	C	VAL B 361	6.793	2.100	30.167	1.00	19.47	B
ATOM	5645	O	VAL B 361	7.232	1.362	31.038	1.00	16.90	B
ATOM	5646	N	MET B 362	5.737	2.885	30.318	1.00	20.10	B
ATOM	5647	CA	MET B 362	4.962	2.882	31.540	1.00	21.78	B
ATOM	5648	CB	MET B 362	4.226	4.206	31.682	1.00	24.19	B
ATOM	5649	CG	MET B 362	3.918	4.589	33.122	1.00	27.23	B
ATOM	5650	SD	MET B 362	5.405	4.806	34.163	1.00	29.11	B
ATOM	5651	CE	MET B 362	4.575	4.880	35.731	1.00	30.05	B
ATOM	5652	C	MET B 362	3.949	1.731	31.471	1.00	20.28	B
ATOM	5653	O	MET B 362	3.385	1.438	30.410	1.00	19.68	B
ATOM	5654	N	PRO B 363	3.698	1.069	32.599	1.00	20.71	B
ATOM	5655	CD	PRO B 363	4.521	1.025	33.818	1.00	21.21	B
ATOM	5656	CA	PRO B 363	2.729	-0.038	32.579	1.00	20.67	B
ATOM	5657	CB	PRO B 363	3.155	-0.883	33.776	1.00	22.57	B
ATOM	5658	CG	PRO B 363	3.665	0.160	34.754	1.00	22.37	B
ATOM	5659	C	PRO B 363	1.272	0.395	32.672	1.00	22.28	B
ATOM	5660	O	PRO B 363	0.959	1.574	32.811	1.00	18.47	B
ATOM	5661	N	MET B 364	0.368	-0.568	32.537	1.00	23.87	B
ATOM	5662	CA	MET B 364	-1.037	-0.272	32.674	1.00	26.94	B
ATOM	5663	CB	MET B 364	-1.780	-0.391	31.332	1.00	29.59	B
ATOM	5664	CG	MET B 364	-1.636	-1.670	30.568	1.00	31.24	B
ATOM	5665	SD	MET B 364	-2.386	-1.510	28.872	1.00	31.43	B

Figure 1 (continued 57)

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ATOM   5666  CE   MET B 364    -4.155   -1.253  29.308  1.00  32.24      B
ATOM   5667  C    MET B 364    -1.602   -1.218  33.725  1.00  30.19      B
ATOM   5668  O    MET B 364    -0.999   -2.251  34.035  1.00  29.20      B
ATOM   5669  N    ARG B 365    -2.732   -0.836  34.307  1.00  32.96      B
ATOM   5670  CA   ARG B 365    -3.383   -1.655  35.324  1.00  36.74      B
ATOM   5671  CB   ARG B 365    -4.029   -0.756  36.394  1.00  37.59      B
ATOM   5672  CG   ARG B 365    -4.785   -1.490  37.505  1.00  39.77      B
ATOM   5673  CD   ARG B 365    -3.859   -2.316  38.398  1.00  40.23      B
ATOM   5674  NE   ARG B 365    -4.571   -2.956  39.505  1.00  40.59      B
ATOM   5675  CZ   ARG B 365    -3.984   -3.707  40.434  1.00  40.64      B
ATOM   5676  NH1  ARG B 365    -2.678   -3.913  40.385  1.00  41.51      B
ATOM   5677  NH2  ARG B 365    -4.698   -4.247  41.418  1.00  41.53      B
ATOM   5678  C    ARG B 365    -4.459   -2.492  34.648  1.00  39.32      B
ATOM   5679  O    ARG B 365    -5.449   -1.961  34.150  1.00  39.51      B
ATOM   5680  N    LEU B 366    -4.267   -3.801  34.609  1.00  41.59      B
ATOM   5681  CA   LEU B 366    -5.272   -4.665  33.996  1.00  44.25      B
ATOM   5682  CB   LEU B 366    -4.615   -5.908  33.366  1.00  45.24      B
ATOM   5683  CG   LEU B 366    -3.640   -5.701  32.202  1.00  45.46      B
ATOM   5684  CD1  LEU B 366    -4.331   -5.029  31.031  1.00  47.09      B
ATOM   5685  CD2  LEU B 366    -2.489   -4.856  32.678  1.00  46.71      B
ATOM   5686  C    LEU B 366    -6.263   -5.080  35.092  1.00  45.55      B
ATOM   5687  O    LEU B 366    -6.424   -6.296  35.333  1.00  46.32      B
ATOM   5688  OXT  LEU B 366    -6.868   -4.169  35.704  1.00  46.33      B
ATOM   5689  CB   ARG C  10    -5.663    0.205  32.737  0.76  34.47      C
ATOM   5690  CG   ARG C  10    -7.073   -0.397  32.771  0.76  36.85      C
ATOM   5691  CD   ARG C  10    -7.748   -0.383  31.408  0.76  39.56      C
ATOM   5692  NE   ARG C  10    -8.728   -1.462  31.268  0.76  41.14      C
ATOM   5693  CZ   ARG C  10    -9.992   -1.301  30.875  0.76  41.65      C
ATOM   5694  NH1  ARG C  10   -10.464   -0.093  30.582  0.76  41.65      C
ATOM   5695  NH2  ARG C  10   -10.779   -2.365  30.749  0.76  42.22      C
ATOM   5696  C    ARG C  10    -4.106    2.152  32.497  0.76  29.83      C
ATOM   5697  O    ARG C  10    -3.278    1.863  33.369  0.76  26.71      C
ATOM   5698  N    ARG C  10    -6.417    2.186  31.464  0.76  33.45      C
ATOM   5699  CA   ARG C  10    -5.587    1.727  32.625  0.76  31.94      C
ATOM   5700  N    GLN C  11    -3.805    2.853  31.408  0.76  28.04      C
ATOM   5701  CA   GLN C  11    -2.458    3.321  31.094  0.76  25.66      C
ATOM   5702  CB   GLN C  11    -2.423    3.866  29.662  0.76  24.07      C
ATOM   5703  CG   GLN C  11    -1.047    4.361  29.231  0.76  21.39      C
ATOM   5704  CD   GLN C  11    -0.039    3.245  29.174  0.76  22.59      C
ATOM   5705  OE1  GLN C  11    -0.263    2.232  28.494  0.76  19.54      C
ATOM   5706  NE2  GLN C  11     1.082    3.415  29.876  0.76  21.15      C
ATOM   5707  C    GLN C  11    -1.895    4.396  32.038  0.76  25.33      C
ATOM   5708  O    GLN C  11    -2.494    5.467  32.217  0.76  25.97      C
ATOM   5709  N    LEU C  12    -0.732    4.111  32.618  0.76  24.73      C
ATOM   5710  CA   LEU C  12    -0.065    5.046  33.519  0.76  25.25      C
ATOM   5711  CB   LEU C  12     0.754    4.277  34.561  0.76  24.93      C
ATOM   5712  CG   LEU C  12    -0.036    3.305  35.450  0.76  23.68      C
ATOM   5713  CD1  LEU C  12     0.907    2.681  36.468  0.76  25.75      C
ATOM   5714  CD2  LEU C  12    -1.184    4.040  36.153  0.76  25.66      C
ATOM   5715  C    LEU C  12     0.845    5.948  32.680  0.76  25.12      C
ATOM   5716  O    LEU C  12     1.111    5.653  31.510  0.76  25.73      C
ATOM   5717  N    VAL C  13     1.317    7.044  33.273  0.76  25.64      C
ATOM   5718  CA   VAL C  13     2.166    7.987  32.543  0.76  25.65      C
ATOM   5719  CB   VAL C  13     1.473    9.371  32.386  0.76  26.39      C
ATOM   5720  CG1  VAL C  13     0.217    9.239  31.523  0.76  26.34      C
ATOM   5721  CG2  VAL C  13     1.113    9.929  33.750  0.76  26.38      C
ATOM   5722  C    VAL C  13     3.542    8.211  33.174  0.76  26.02      C
ATOM   5723  O    VAL C  13     3.740    8.050  34.381  0.76  24.85      C
ATOM   5724  N    LEU C  14     4.498    8.596  32.339  0.76  26.90      C
ATOM   5725  CA   LEU C  14     5.860    8.846  32.803  0.76  28.40      C
ATOM   5726  CB   LEU C  14     6.836    8.819  31.619  0.76  28.31      C
ATOM   5727  CG   LEU C  14     6.972    7.481  30.889  0.76  29.36      C
ATOM   5728  CD1  LEU C  14     7.666    7.705  29.557  0.76  30.19      C
ATOM   5729  CD2  LEU C  14     7.744    6.495  31.769  0.76  29.17      C
ATOM   5730  C    LEU C  14     6.010   10.186  33.517  0.76  29.12      C
ATOM   5731  O    LEU C  14     5.238   11.126  33.284  0.76  29.91      C
ATOM   5732  N    GLY C  15     7.000   10.263  34.396  0.76  29.70      C
ATOM   5733  CA   GLY C  15     7.264   11.510  35.090  0.76  32.11      C
ATOM   5734  C    GLY C  15     8.263   12.275  34.234  0.76  33.78      C
ATOM   5735  O    GLY C  15     9.472   12.210  34.462  0.76  35.30      C
ATOM   5736  N    LEU C  16     7.750   12.995  33.241  0.76  34.34      C
ATOM   5737  CA   LEU C  16     8.576   13.756  32.306  0.76  34.95      C
ATOM   5738  CB   LEU C  16     7.732   14.157  31.094  0.76  33.39      C
ATOM   5739  CG   LEU C  16     7.258   12.955  30.269  0.76  30.69      C
ATOM   5740  CD1  LEU C  16     6.303   13.411  29.171  0.76  30.83      C
ATOM   5741  CD2  LEU C  16     8.467   12.233  29.690  0.76  31.29      C
ATOM   5742  C    LEU C  16     9.263   14.982  32.898  0.76  36.04      C
ATOM   5743  O    LEU C  16    10.182   15.515  32.231  0.76  36.84      C
ATOM   5744  OXT  LEU C  16     8.870   15.398  34.009  0.76  37.64      C
ATOM   5745  OH2  TIP S   1    -4.929  -23.609  18.052  1.00  15.99      S
ATOM   5746  OH2  TIP S   2     4.228    8.274 -26.027  1.00  13.10      S
ATOM   5747  OH2  TIP S   3    10.558   12.623 -25.084  1.00  15.30      S
ATOM   5748  OH2  TIP S   4     5.227  -21.550  19.916  1.00  15.79      S
ATOM   5749  OH2  TIP S   5     8.098   19.305 -28.222  1.00  16.24      S
ATOM   5750  OH2  TIP S   6    15.241   27.169  -6.212  1.00  15.04      S
ATOM   5751  OH2  TIP S   7    20.667   23.747 -19.701  1.00  12.11      S
ATOM   5752  OH2  TIP S   8     8.057  -16.814  20.553  1.00  18.56      S
ATOM   5753  OH2  TIP S   9    -8.202   -7.752 -28.805  1.00  15.40      S
ATOM   5754  OH2  TIP S  10    -3.188   14.555 -36.202  1.00  15.80      S
ATOM   5755  OH2  TIP S  11    -8.735   18.253 -21.735  1.00  16.46      S
ATOM   5756  OH2  TIP S  12     1.707    0.243  28.691  1.00  19.43      S
ATOM   5757  OH2  TIP S  13    21.827   20.941 -18.878  1.00  15.07      S
ATOM   5758  OH2  TIP S  14   -12.919    1.529 -20.565  1.00  14.60      S
ATOM   5759  OH2  TIP S  15     6.506    7.845 -24.491  1.00  14.11      S
ATOM   5760  OH2  TIP S  16   -16.095  -26.586   6.640  1.00  18.29      S
ATOM   5761  OH2  TIP S  17   -20.810   -5.324 -15.729  1.00  15.06      S
ATOM   5762  OH2  TIP S  18     6.790  -16.969  34.740  1.00  14.72      S
ATOM   5763  OH2  TIP S  19   -28.633  -22.763  -9.122  1.00  19.48      S
ATOM   5764  OH2  TIP S  20    -4.575   19.633 -14.656  1.00  16.85      S
ATOM   5765  OH2  TIP S  21     6.941    2.131  23.109  1.00  18.16      S
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Figure 1 (continued 58)

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ATOM    5766  OH2 TIP S  22     -27.660 -14.486 -13.561  1.00 17.12          S
ATOM    5767  OH2 TIP S  23     -13.962  -0.925 -21.605  1.00 14.22          S
ATOM    5768  OH2 TIP S  24       1.435  28.503 -10.938  1.00 18.48          S
ATOM    5769  OH2 TIP S  25       9.366   3.813  23.519  1.00 16.22          S
ATOM    5770  OH2 TIP S  26       6.434 -22.228  22.332  1.00 19.93          S
ATOM    5771  OH2 TIP S  27       7.890 -18.056  18.119  1.00 19.57          S
ATOM    5772  OH2 TIP S  28     -15.000   8.720 -22.814  1.00 14.68          S
ATOM    5773  OH2 TIP S  29      10.776  24.804 -24.045  1.00 16.80          S
ATOM    5774  OH2 TIP S  30       1.778  20.791  -6.653  1.00 17.56          S
ATOM    5775  OH2 TIP S  31       0.621  20.501  -9.333  1.00 18.49          S
ATOM    5776  OH2 TIP S  32       4.572   1.385 -28.353  1.00 18.53          S
ATOM    5777  OH2 TIP S  33       8.530  13.438  21.012  1.00 18.38          S
ATOM    5778  OH2 TIP S  34      -5.364 -34.951  13.172  1.00 16.54          S
ATOM    5779  OH2 TIP S  35      -0.215  -6.534 -30.846  1.00 17.23          S
ATOM    5780  OH2 TIP S  36       3.783  18.454 -29.707  1.00 19.51          S
ATOM    5781  OH2 TIP S  37       3.591  -1.199 -27.445  1.00 19.45          S
ATOM    5782  OH2 TIP S  38       9.369  34.981 -11.888  1.00 20.02          S
ATOM    5783  OH2 TIP S  39      10.133 -20.154  36.900  1.00 17.90          S
ATOM    5784  OH2 TIP S  40       3.793   8.403 -19.080  1.00 16.65          S
ATOM    5785  OH2 TIP S  41      10.939   4.680  14.536  1.00 18.20          S
ATOM    5786  OH2 TIP S  42       8.076  12.297 -25.798  1.00 16.16          S
ATOM    5787  OH2 TIP S  43     -14.372 -32.728   6.563  1.00 18.38          S
ATOM    5788  OH2 TIP S  44     -23.715  -9.227 -23.646  1.00 21.11          S
ATOM    5789  OH2 TIP S  45      20.825  28.255  -9.159  1.00 16.67          S
ATOM    5790  OH2 TIP S  46      -1.109  13.957 -40.824  1.00 17.50          S
ATOM    5791  OH2 TIP S  47       5.330 -27.571  17.233  1.00 20.27          S
ATOM    5792  OH2 TIP S  48      -6.283  -7.101  26.866  1.00 19.83          S
ATOM    5793  OH2 TIP S  49      -4.904  -9.220  29.033  1.00 18.63          S
ATOM    5794  OH2 TIP S  50       6.596  25.027  -2.197  1.00 18.25          S
ATOM    5795  OH2 TIP S  51       3.946 -28.513  19.328  1.00 22.98          S
ATOM    5796  OH2 TIP S  52      18.496  30.057  13.872  1.00 21.35          S
ATOM    5797  OH2 TIP S  53      14.476  13.406 -26.031  1.00 20.88          S
ATOM    5798  OH2 TIP S  54      -5.854  17.119 -30.322  1.00 18.67          S
ATOM    5799  OH2 TIP S  55     -11.444 -12.723  13.885  1.00 21.78          S
ATOM    5800  OH2 TIP S  56     -18.531 -23.945  -2.069  1.00 20.92          S
ATOM    5801  OH2 TIP S  57       8.793  -1.749  36.685  1.00 23.51          S
ATOM    5802  OH2 TIP S  58     -10.518  17.199 -18.634  1.00 19.66          S
ATOM    5803  OH2 TIP S  59      18.320  33.650 -11.778  1.00 23.35          S
ATOM    5804  OH2 TIP S  60       3.811  10.767 -14.624  1.00 21.33          S
ATOM    5805  OH2 TIP S  61      10.630 -17.965  40.549  1.00 20.18          S
ATOM    5806  OH2 TIP S  62       7.563  12.545 -28.560  1.00 22.05          S
ATOM    5807  OH2 TIP S  63      17.504  24.804   2.515  1.00 17.88          S
ATOM    5808  OH2 TIP S  64      11.187   4.750 -21.381  1.00 18.39          S
ATOM    5809  OH2 TIP S  65       3.669  23.465   0.736  1.00 20.78          S
ATOM    5810  OH2 TIP S  66       0.642 -25.439  24.271  1.00 19.92          S
ATOM    5811  OH2 TIP S  67      -5.697 -28.454  21.972  1.00 20.88          S
ATOM    5812  OH2 TIP S  68       4.514  12.181 -28.340  1.00 18.14          S
ATOM    5813  OH2 TIP S  69     -20.340 -23.019  19.925  1.00 21.76          S
ATOM    5814  OH2 TIP S  70       1.000  -3.521  35.944  1.00 23.02          S
ATOM    5815  OH2 TIP S  71       4.561  34.315 -12.922  1.00 19.38          S
ATOM    5816  OH2 TIP S  72     -20.556   2.785 -36.420  1.00 27.46          S
ATOM    5817  OH2 TIP S  73       4.764  -1.117 -32.012  1.00 27.35          S
ATOM    5818  OH2 TIP S  74     -20.786 -26.799  16.978  1.00 21.37          S
ATOM    5819  OH2 TIP S  75      30.429  23.473  16.248  1.00 26.87          S
ATOM    5820  OH2 TIP S  76     -14.593  15.544 -36.291  1.00 26.66          S
ATOM    5821  OH2 TIP S  77      27.307  15.098   1.258  1.00 25.86          S
ATOM    5822  OH2 TIP S  78       5.319   7.976 -32.697  1.00 23.44          S
ATOM    5823  OH2 TIP S  79       8.457 -24.862  15.056  1.00 27.61          S
ATOM    5824  OH2 TIP S  80      -0.400  -9.335  16.470  1.00 23.64          S
ATOM    5825  OH2 TIP S  81     -30.824 -24.685  -8.816  1.00 23.87          S
ATOM    5826  OH2 TIP S  82      -2.412  16.657 -12.786  1.00 22.67          S
ATOM    5827  OH2 TIP S  83     -16.348   6.876 -33.518  1.00 30.01          S
ATOM    5828  OH2 TIP S  84      -4.781  13.922 -43.086  1.00 19.96          S
ATOM    5829  OH2 TIP S  85      22.867  14.713  -4.352  1.00 27.67          S
ATOM    5830  OH2 TIP S  86      14.019  34.958 -17.016  1.00 24.03          S
ATOM    5831  OH2 TIP S  87     -22.863  -7.339  -7.089  1.00 30.51          S
ATOM    5832  OH2 TIP S  88       0.014 -13.197  13.132  1.00 24.07          S
ATOM    5833  OH2 TIP S  89      -0.477 -26.421  26.641  1.00 22.63          S
ATOM    5834  OH2 TIP S  90       8.749   0.467  15.868  1.00 29.65          S
ATOM    5835  OH2 TIP S  91      -6.197  -6.594  19.747  1.00 23.37          S
ATOM    5836  OH2 TIP S  92       7.703   5.467 -24.148  1.00 20.70          S
ATOM    5837  OH2 TIP S  93       1.486 -22.220  27.625  1.00 23.06          S
ATOM    5838  OH2 TIP S  94      -8.748  -9.800  20.699  1.00 22.04          S
ATOM    5839  OH2 TIP S  95     -16.624   1.189 -13.898  1.00 21.62          S
ATOM    5840  OH2 TIP S  96     -17.781  -3.404 -34.492  1.00 24.71          S
ATOM    5841  OH2 TIP S  97      22.028  14.095 -22.382  1.00 22.02          S
ATOM    5842  OH2 TIP S  98       0.850  24.987 -25.136  1.00 29.29          S
ATOM    5843  OH2 TIP S  99       3.761  -8.089  41.138  1.00 24.22          S
ATOM    5844  OH2 TIP S 100       6.060 -19.622  23.723  1.00 20.71          S
ATOM    5845  OH2 TIP S 101     -20.830  -8.439  -5.124  1.00 25.02          S
ATOM    5846  OH2 TIP S 102     -23.978 -22.857 -27.649  1.00 27.37          S
ATOM    5847  OH2 TIP S 103     -19.110 -26.350   4.119  1.00 28.04          S
ATOM    5848  OH2 TIP S 104     -10.419  10.168 -16.512  1.00 20.89          S
ATOM    5849  OH2 TIP S 106      26.620   6.278   5.868  1.00 26.84          S
ATOM    5850  OH2 TIP S 107      15.079 -16.710  41.044  1.00 31.49          S
ATOM    5851  OH2 TIP S 108      -6.608  -4.481  27.748  1.00 21.60          S
ATOM    5852  OH2 TIP S 109     -10.514  -6.785  27.903  1.00 28.76          S
ATOM    5853  OH2 TIP S 110       7.483  34.057 -13.520  1.00 20.71          S
ATOM    5854  OH2 TIP S 111      -6.501 -31.759  -5.806  1.00 31.23          S
ATOM    5855  OH2 TIP S 112      -2.508  -7.957  17.238  1.00 28.35          S
ATOM    5856  OH2 TIP S 113     -16.554   3.360 -34.120  1.00 19.83          S
ATOM    5857  OH2 TIP S 114      -1.472  10.711 -15.764  1.00 27.87          S
ATOM    5858  OH2 TIP S 115     -22.960 -28.887 -19.727  1.00 25.60          S
ATOM    5859  OH2 TIP S 116      15.115 -14.901  19.731  1.00 24.51          S
ATOM    5860  OH2 TIP S 117      -5.148 -33.100  -3.606  1.00 25.41          S
ATOM    5861  OH2 TIP S 118      20.099  -0.396  23.402  1.00 22.68          S
ATOM    5862  OH2 TIP S 119      -7.111  -2.117 -16.703  1.00 24.27          S
ATOM    5863  OH2 TIP S 120     -11.193  -9.224  19.755  1.00 25.30          S
ATOM    5864  OH2 TIP S 121      18.193 -11.449  36.973  1.00 27.57          S
ATOM    5865  OH2 TIP S 122     -22.357   2.771 -13.647  1.00 25.49
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Figure 1 (continued 59)

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ATOM   5866   OH2 TIP S 123      20.077   32.381   13.831   1.00 28.68        S
ATOM   5867   OH2 TIP S 124     -17.741    4.784  -15.367   1.00 27.89        S
ATOM   5868   OH2 TIP S 125       4.106  -14.005   15.492   1.00 25.37        S
ATOM   5869   OH2 TIP S 126      13.838   16.125  -26.991   1.00 25.20        S
ATOM   5870   OH2 TIP S 127      -2.287  -34.498    8.522   1.00 26.09        S
ATOM   5871   OH2 TIP S 128     -11.663   -6.092   22.298   1.00 28.13        S
ATOM.  5872   OH2 TIP S 129      11.561   18.821  -28.755   1.00 36.46        S
ATOM   5873   OH2 TIP S 130       7.031    1.863  -26.963   1.00 26.76        S
ATOM   5874   OH2 TIP S 131       6.205  -28.726    8.902   1.00 29.30        S
ATOM   5875   OH2 TIP S 132     -10.559   19.568  -19.983   1.00 20.77        S
ATOM   5876   OH2 TIP S 133      22.972   19.220  -17.034   1.00 20.45        S
ATOM   5877   OH2 TIP S 134       5.249   21.787    8.628   1.00 29.10        S
ATOM   5878   OH2 TIP S 135      16.410   14.232   27.045   1.00 27.03        S
ATOM   5879   OH2 TIP S 136      -3.218  -34.687   11.046   1.00 24.07        S
ATOM   5880   OH2 TIP S 137      24.833   28.261  -21.884   1.00 22.96        S
ATOM   5881   OH2 TIP S 138      13.264   35.476  -14.774   1.00 30.23        S
ATOM   5882   OH2 TIP S 139      -2.053    2.392   26.549   1.00 25.03        S
ATOM   5883   OH2 TIP S 140      11.605   15.067    0.133   1.00 34.22        S
ATOM   5884   OH2 TIP S 141      13.972   24.010   19.832   1.00 25.81        S
ATOM   5885   OH2 TIP S 142     -19.355  -25.503   19.026   1.00 29.46        S
ATOM   5886   OH2 TIP S 143      -4.006  -31.965    2.763   1.00 26.41        S
ATOM   5887   OH2 TIP S 144      15.901   28.652   -2.514   1.00 25.23        S
ATOM   5888   OH2 TIP S 145     -17.355  -32.497   18.572   1.00 25.07        S
ATOM.  5889   OH2 TIP S 146       0.958  -13.688   32.466   1.00 22.13        S
ATOM   5890   OH2 TIP S 147      -6.459   12.128  -44.255   1.00 32.10        S
ATOM   5891   OH2 TIP S 148      -0.707  -24.653    2.977   1.00 26.54        S
ATOM   5892   OH2 TIP S 149     -12.838  -12.951   11.427   1.00 23.90        S
ATOM   5893   OH2 TIP S 150     -24.404  -11.780  -24.495   1.00 25.54        S
ATOM   5894   OH2 TIP S 151       0.539   -6.289  -33.601   1.00 29.88        S
ATOM   5895   OH2 TIP S 152     -13.161  -28.396   -0.606   1.00 27.46        S
ATOM   5896   OH2 TIP S 153      10.877    9.824    5.701   1.00 24.98        S
ATOM   5897   OH2 TIP S 154     -24.429  -25.832    1.552   1.00 29.48        S
ATOM   5898   OH2 TIP S 155       9.976   29.261    3.159   1.00 26.39        S
ATOM   5899   OH2 TIP S 156      -8.594   -7.245  -13.161   1.00 38.12        S
ATOM   5900   OH2 TIP S 157       2.066   24.920    5.025   1.00 22.77        S
ATOM   5901   OH2 TIP S 158     -15.909   14.296  -28.353   1.00 25.22        S
ATOM   5902   OH2 TIP S 159       0.091   16.467  -11.319   1.00 24.31        S
ATOM   5903   OH2 TIP S 160      16.526  -12.797   18.583   1.00 26.81        S
ATOM   5904   OH2 TIP S 161       3.049    7.864   19.831   1.00 24.57        S
ATOM   5905   OH2 TIP S 162      21.865   -8.253   21.271   1.00 23.66        S
ATOM   5906   OH2 TIP S 163      -7.960   -6.892  -33.834   1.00 30.32        S
ATOM   5907   OH2 TIP S 164      19.362  -16.854   36.055   1.00 31.05        S
ATOM   5908   OH2 TIP S 165      -5.308  -32.390   18.952   1.00 29.57        S
ATOM   5909   OH2 TIP S 166     -11.933  -29.026   -5.229   1.00 26.58        S
ATOM   5910   OH2 TIP S 167     -19.093  -31.089   17.480   1.00 33.54        S
ATOM   5911   OH2 TIP S 168      14.092   18.448  -25.956   1.00 29.46        S
ATOM   5912   OH2 TIP S 169      10.876    5.438   12.054   1.00 32.82        S
ATOM   5913   OH2 TIP S 170      -6.890   -9.072  -26.532   1.00 25.82        S
ATOM   5914   OH2 TIP S 171      29.867   28.203   18.182   1.00 30.29        S
ATOM   5915   OH2 TIP S 172      16.406   39.004    9.209   1.00 28.96        S
ATOM   5916   OH2 TIP S 173      -4.013  -11.245   30.748   1.00 25.90        S
ATOM   5917   OH2 TIP S 174     -26.979  -31.890   -8.368   1.00 36.88        S
ATOM   5918   OH2 TIP S 175     -23.390    1.597  -33.916   1.00 36.95        S
ATOM   5919   OH2 TIP S 176     -21.827  -20.068   21.374   1.00 28.64        S
ATOM   5920   OH2 TIP S 177     -17.123  -16.612    7.118   1.00 25.01        S
ATOM   5921   OH2 TIP S 178      -0.586   30.510  -11.769   1.00 23.24        S
ATOM   5922   OH2 TIP S 179       6.159   20.259   17.337   1.00 30.73        S
ATOM   5923   OH2 TIP S 180      21.260   -1.762   19.163   1.00 34.09        S
ATOM   5924   OH2 TIP S 181      -2.864  -28.282    2.753   1.00 27.53        S
ATOM   5925   OH2 TIP S 182      -8.835  -11.179   -6.743   1.00 29.61        S
ATOM   5926   OH2 TIP S 183      15.829   24.884  -23.368   1.00 31.33        S
ATOM   5927   OH2 TIP S 184      24.002   17.831  -10.733   1.00 29.65        S
ATOM   5928   OH2 TIP S 185     -29.401    5.440  -14.949   1.00 32.48        S
ATOM   5929   OH2 TIP S 186      -1.383  -33.459   19.317   1.00 29.25        S
ATOM   5930   OH2 TIP S 187      12.063  -19.966   25.080   1.00 25.65        S
ATOM   5931   OH2 TIP S 188      -4.351   -9.679  -26.788   1.00 27.17        S
ATOM   5932   OH2 TIP S 189       3.729    5.832   16.486   1.00 34.24        S
ATOM   5933   OH2 TIP S 190       9.565   37.434   -9.975   1.00 27.30        S
ATOM   5934   OH2 TIP S 191       1.483   14.975  -40.508   1.00 31.36        S
ATOM   5935   OH2 TIP S 192      -6.648  -10.961  -20.165   1.00 32.28        \S
ATOM   5936   OH2 TIP S 193       3.745   12.221   31.113   1.00 29.48        S
ATOM   5937   OH2 TIP S 194       2.400  -29.701  -15.849   1.00 26.51        S
ATOM   5938   OH2 TIP S 195       1.145  -29.287   18.977   1.00 27.97        S
ATOM   5939   OH2 TIP S 196       1.173   24.321  -30.127   1.00 37.69        S
ATOM   5940   OH2 TIP S 197     -28.254  -20.580    5.716   1.00 43.95        S
ATOM   5941   OH2 TIP S 198      22.283   20.039   25.715   1.00 34.76        S
ATOM   5942   OH2 TIP S 199      -1.895    4.664  -43.775   1.00 27.75        S
ATOM   5943   OH2 TIP S 200      23.429   31.198  -15.860   1.00 32.99        S
ATOM   5944   OH2 TIP S 201      -9.479   -5.901  -15.419   1.00 21.16        S
ATOM   5945   OH2 TIP S 202     -12.878    0.162  -12.723   1.00 33.84        S
ATOM   5946   OH2 TIP S 203       5.581   19.187   14.793   1.00 27.97        S
ATOM   5947   OH2 TIP S 204     -23.954  -24.578   -2.262   1.00 30.51        S
ATOM   5948   OH2 TIP S 205       3.457   33.211  -23.268   1.00 31.98        S
ATOM   5949   OH2 TIP S 206     -17.263    0.457  -42.268   1.00 31.49        S
ATOM   5950   OH2 TIP S 207      16.260   31.888    2.413   1.00 23.24        S
ATOM   5951   OH2 TIP S 208      -4.320    1.145   26.565   1.00 29.38        S
ATOM   5952   OH2 TIP S 209     -19.947    2.160  -11.744   1.00 38.41        S
ATOM   5953   OH2 TIP S 210       1.872   26.689  -27.041   1.00 29.78        S
ATOM   5954   OH2 TIP S 211     -13.714   23.099  -13.845   1.00 33.77        S
ATOM   5955   OH2 TIP S 212       9.218   35.580  -19.331   1.00 29.22        S
ATOM   5956   OH2 TIP S 213      -0.219   26.259    5.173   1.00 31.76        S
ATOM   5957   OH2 TIP S 214      -8.272    3.938  -13.966   1.00 35.25        S
ATOM   5958   OH2 TIP S 215       9.984  -22.548   31.867   1.00 33.85        S
ATOM   5959   OH2 TIP S 216     -30.386  -28.425    2.476   1.00 30.05        S
ATOM   5960   OH2 TIP S 217       5.272   16.545  -36.105   1.00 33.30        S
ATOM   5961   OH2 TIP S 218     -14.957   -2.170  -39.231   1.00 30.96        S
ATOM   5962   OH2 TIP S 219       2.136  -28.546   23.097   1.00 39.83        S
ATOM   5963   OH2 TIP S 220       0.866   11.873   23.871   1.00 32.14        S
ATOM   5964   OH2 TIP S 221      -7.469   -8.003  -23.367   1.00 24.79        S
ATOM   5965   OH2 TIP S 222      10.219    6.251   34.646   1.00 37.06        S
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Figure 1 (continued 60)

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ATOM   5966  OH2 TIP S 223       9.603 -19.191   12.099  1.00 30.03          S
ATOM   5967  OH2 TIP S 224      15.592   1.270   14.898  1.00 29.33          S
ATOM   5968  OH2 TIP S 225      -7.625 -22.611  -22.802  1.00 32.63          S
ATOM   5969  OH2 TIP S 226     -30.236 -24.968  -11.543  1.00 24.51          S
ATOM   5970  OH2 TIP S 227     -11.748 -27.136   28.999  1.00 35.80          S
ATOM   5971  OH2 TIP S 228     -17.912 -19.364   23.072  1.00 31.69          S
ATOM   5972  OH2 TIP S 229     -12.001   4.279  -15.335  1.00 28.59          S
ATOM   5973  OH2 TIP S 230      27.573  31.316   11.831  1.00 32.14          S
ATOM   5974  OH2 TIP S 231     -25.350   3.037  -21.957  1.00 30.50          S
ATOM   5975  OH2 TIP S 232      -9.948  19.698  -27.138  1.00 32.26          S
ATOM   5976  OH2 TIP S 233      31.351  11.309   12.566  1.00 40.60          S
ATOM   5977  OH2 TIP S 234       7.345   8.147   -8.973  1.00 40.15          S
ATOM   5978  OH2 TIP S 235      13.323  25.650  -24.378  1.00 28.39          S
ATOM   5979  OH2 TIP S 236      14.326 -23.002   38.347  1.00 44.20          S
ATOM   5980  OH2 TIP S 237      18.205  35.226  -19.376  1.00 36.69          S
ATOM   5981  OH2 TIP S 238       7.073   7.343  -21.458  1.00 26.18          S
ATOM   5982  OH2 TIP S 239       6.134 -17.380   11.852  1.00 34.32          S
ATOM   5983  OH2 TIP S 240      -6.807   3.536  -42.001  1.00 25.28          S
ATOM   5984  OH2 TIP S 241     -24.937 -17.863  -25.603  1.00 32.04          S
ATOM   5985  OH2 TIP S 242     -17.088 -21.664  -30.797  1.00 30.50          S
ATOM   5986  OH2 TIP S 243       6.771  -7.663   14.406  1.00 36.01          S
ATOM   5987  OH2 TIP S 244     -27.706 -30.578   -5.708  1.00 47.96          S
ATOM   5988  OH2 TIP S 245     -21.059  10.316  -25.562  1.00 35.65          S
ATOM   5989  OH2 TIP S 246      10.606  28.216  -25.525  1.00 29.43          S
ATOM   5990  OH2 TIP S 247       1.528   5.171  -17.593  1.00 27.85          S
ATOM   5991  OH2 TIP S 248     -29.012 -18.667  -20.134  1.00 33.27          S
ATOM   5992  OH2 TIP S 249     -21.413 -24.799    4.888  1.00 34.44          S
ATOM   5993  OH2 TIP S 250       1.196  -8.297  -29.245  1.00 27.57          S
ATOM   5994  OH2 TIP S 251      -0.162 -13.772   35.108  1.00 36.60          S
ATOM   5995  OH2 TIP S 252      19.156 -15.454   21.696  1.00 29.04          S
ATOM   5996  OH2 TIP S 253      21.723  17.101  -18.745  1.00  9.13          S
ATOM   5997  OH2 TIP S 254       7.667   9.573  -26.321  1.00 15.05          S
ATOM   5998  OH2 TIP S 255       5.459   9.537  -28.155  1.00 14.20          S
ATOM   5999  OH2 TIP S 256       7.583 -20.372   19.535  1.00 17.45          S
ATOM   6000  OH2 TIP S 257       8.434   5.091  -21.601  1.00 20.19          S
ATOM   6001  OH2 TIP S 258      10.303 -20.727   39.479  1.00 21.19          S
ATOM   6002  OH2 TIP S 259      23.351  15.777  -20.932  1.00 24.25          S
ATOM   6003  OH2 TIP S 260       8.255 -19.223   21.937  1.00 16.91          S
ATOM   6004  OH2 TIP S 261       7.407  21.555  -29.683  1.00 18.42          S
ATOM   6005  OH2 TIP S 262       0.133 -33.614    9.571  1.00 23.67          S
ATOM   6006  OH2 TIP S 263       1.067  23.311  -27.412  1.00 26.04          S
ATOM   6007  OH2 TIP S 264      10.172 -20.657   23.070  1.00 20.75          S
ATOM   6008  OH2 TIP S 265       5.434   1.347  -31.078  1.00 25.19          S
ATOM   6009  OH2 TIP S 266       6.473   8.791  -30.462  1.00 22.73          S
ATOM   6010  OH2 TIP S 267      16.690 -16.534   21.428  1.00 23.86          S
ATOM   6011  OH2 TIP S 268      -7.886  21.056  -13.245  1.00 26.88          S
ATOM   6012  OH2 TIP S 269      12.771  20.121  -27.176  1.00 33.96          S
ATOM   6013  OH2 TIP S 270     -17.226   9.655  -21.614  1.00 26.62          S
ATOM   6014  OH2 TIP S 271      -2.213  14.948  -43.167  1.00 24.56          S
ATOM   6015  OH2 TIP S 272       9.664   5.525  -25.968  1.00 25.69          S
ATOM   6016  OH2 TIP S 273       6.917 -25.402   17.512  1.00 27.80          S
ATOM   6017  OH2 TIP S 274      -4.242 -20.885   28.965  1.00 32.23          S
ATOM   6018  OH2 TIP S 275     -17.221 -17.062   17.975  1.00 28.09          S
ATOM   6019  OH2 TIP S 276      12.668  11.417  -26.228  1.00 27.75          S
ATOM   6020  OH2 TIP S 277      10.299   1.950   14.305  1.00 27.65          S
ATOM   6021  OH2 TIP S 278     -31.806 -30.359   -6.948  1.00 57.47          S
ATOM   6022  OH2 TIP S 279     -26.463   4.339   -9.507  1.00 29.65          S
ATOM   6023  OH2 TIP S 280     -26.015 -34.574   -7.677  1.00 26.06          S
ATOM   6024  OH2 TIP S 281     -31.347   5.379  -17.218  1.00 33.42          S
ATOM   6025  OH2 TIP S 282      14.453 -16.744   17.668  1.00 30.41          S
ATOM   6026  OH2 TIP S 283      27.710   8.976    5.055  1.00 26.81          S
ATOM   6027  OH2 TIP S 284       2.896   8.795  -16.720  1.00 27.99          S
ATOM   6028  OH2 TIP S 285      -9.100  19.482  -24.203  1.00 25.80          S
ATOM   6029  OH2 TIP S 286      -2.579   1.667   21.500  1.00 29.60          S
ATOM   6030  OH2 TIP S 287       6.335  11.378  -31.555  1.00 29.71          S
ATOM   6031  OH2 TIP S 288      12.371 -16.564   41.802  1.00 31.26          S
ATOM   6032  OH2 TIP S 289       0.360 -29.275   21.468  1.00 31.50          S
ATOM   6033  OH2 TIP S 290      -2.645   4.725   26.240  1.00 33.72          S
ATOM   6034  OH2 TIP S 291      19.718  -0.267   20.338  1.00 32.39         \S
ATOM   6035  OH2 TIP S 292       7.034  29.199    9.979  1.00 29.78         \S
ATOM   6036  OH2 TIP S 293      -4.995  20.991  -12.507  1.00 34.58          S
ATOM   6037  OH2 TIP S 294     -28.086 -24.068  -26.481  1.00 30.52          S
ATOM   6038  OH2 TIP S 295       4.690  32.380  -25.768  1.00 32.16          S
ATOM   6039  OH2 TIP S 296      12.183  37.736   -9.852  1.00 32.44          S
ATOM   6040  OH2 TIP S 297      -0.897  -9.935  -28.834  1.00 28.74          S
ATOM   6041  OH2 TIP S 298      -5.666 -26.946   -3.776  1.00 35.30          S
ATOM   6042  OH2 TIP S 299     -19.121 -17.609   23.997  1.00 30.20          S
ATOM   6043  OH2 TIP S 300      11.846   2.521  -20.488  1.00 34.76          S
ATOM   6044  OH2 TIP S 301      21.299   6.735   24.995  1.00 37.00          S
ATOM   6045  OH2 TIP S 302     -23.638 -27.161   16.432  1.00 29.19          S
ATOM   6046  OH2 TIP S 303       1.556  -0.845  -22.820  1.00 34.60          S
ATOM   6047  OH2 TIP S 304     -12.057 -30.800   -2.592  1.00 30.84          S
ATOM   6048  OH2 TIP S 305      16.694 -19.967   30.452  1.00 32.66          S
ATOM   6049  OH2 TIP S 306       0.157  25.634   -7.191  1.00 32.17          S
ATOM   6050  OH2 TIP S 307      -0.449  27.840  -20.073  1.00 29.18          S
ATOM   6051  OH2 TIP S 308      21.819   3.025    9.910  1.00 41.68          S
ATOM   6052  OH2 TIP S 309     -15.005 -11.439  -28.535  1.00 38.02          S
ATOM   6053  OH2 TIP S 310     -21.942 -31.716   -8.240  1.00 33.01          S
ATOM   6054  OH2 TIP S 311      -8.284 -25.125  -23.593  1.00 41.18          S
ATOM   6055  OH2 TIP S 312       2.515   4.002  -33.125  1.00 26.47          S
ATOM   6056  OH2 TIP S 313     -18.335  13.849  -29.235  1.00 30.43          S
ATOM   6057  OH2 TIP S 314     -12.912  -8.449   21.566  1.00 30.42          S
ATOM   6058  OH2 TIP S 315      -1.397 -26.362    1.310  1.00 33.91          S
ATOM   6059  OH2 TIP S 316       9.366 -22.526   35.732  1.00 30.66          S
ATOM   6060  OH2 TIP S 317     -25.401 -30.023   -8.998  1.00 29.44          S
ATOM   6061  OH2 TIP S 318     -21.887   3.702  -34.234  1.00 36.98          S
ATOM   6062  OH2 TIP S 319      -8.700 -20.782  -24.886  1.00 32.89          S
ATOM   6063  OH2 TIP S 320     -20.333 -29.925   -6.872  1.00 34.64          S
ATOM   6064  OH2 TIP S 321      -7.827 -13.241  -33.387  1.00 32.71          S
ATOM   6065  OH2 TIP S 322      14.750  31.182    9.293  1.00 31.66          S
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Figure 1 (continued 61)

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ATOM   6066  OH2 TIP S 323     -24.400 -19.167  20.554  1.00 30.46      S
ATOM   6067  OH2 TIP S 324      -9.584   3.692 -42.248  1.00 33.30      S
ATOM   6068  OH2 TIP S 325       6.014  19.032 -31.179  1.00 40.38      S
ATOM   6069  OH2 TIP S 326     -13.974 -30.622  -5.965  1.00 32.26      S
ATOM   6070  OH2 TIP S 327     -29.857 -10.593  -7.579  1.00 34.80      S
ATOM   6071  OH2 TIP S 328      12.690  33.497 -20.379  1.00 34.07      S
ATOM   6072  OH2 TIP S 329       7.069   2.658 -20.988  1.00 28.88      S
ATOM   6073  OH2 TIP S 330      12.019  -0.360  36.086  1.00 26.34      S
ATOM   6074  OH2 TIP S 331     -22.705   5.938 -14.330  1.00 34.70      S
ATOM   6075  OH2 TIP S 332       8.097  14.122  -2.649  1.00 39.46      S
ATOM   6076  OH2 TIP S 333     -21.898 -21.927   4.044  1.00 37.81      S
ATOM   6077  OH2 TIP S 334       9.937 -17.771  16.216  1.00 29.70      S
ATOM   6078  OH2 TIP S 335     -16.221  -6.845 -33.678  1.00 33.31      S
ATOM   6079  OH2 TIP S 336      -3.494 -22.898 -17.063  1.00 31.83      S
ATOM   6080  OH2 TIP S 337     -22.157   5.573 -30.240  1.00 39.35      S
ATOM   6081  OH2 TIP S 338      -7.617 -32.398  -8.188  1.00 30.34      S
ATOM   6082  OH2 TIP S 339      23.475  29.150  -8.430  1.00 36.32      S
ATOM   6083  OH2 TIP S 340      -7.276  -9.187 -35.186  1.00 41.69      S
ATOM   6084  OH2 TIP S 341      26.845  32.870   8.481  1.00 37.63      S
ATOM   6085  OH2 TIP S 342     -12.192  21.236 -21.321  1.00 30.21      S
ATOM   6086  OH2 TIP S 343     -14.628 -35.461  19.832  1.00 35.16      S
ATOM   6087  OH2 TIP S 344      -5.653 -31.128  21.101  1.00 34.25      S
ATOM   6088  OH2 TIP S 345      -6.084  -8.172 -19.496  1.00 36.21      S
ATOM   6089  OH2 TIP S 346      27.089  28.347   6.056  1.00 42.19      S
ATOM   6090  OH2 TIP S 347      17.043  22.284 -26.012  1.00 32.12      S
ATOM   6091  OH2 TIP S 348     -21.277   2.842 -26.424  1.00 36.86      S
ATOM   6092  OH2 TIP S 349     -23.886 -14.574 -31.320  1.00 39.26      S
ATOM   6093  OH2 TIP S 350       5.980  19.532  10.965  1.00 26.13      S
ATOM   6094  OH2 TIP S 351      15.574  -9.666  16.201  1.00 35.41      S
ATOM   6095  OH2 TIP S 352     -20.467 -13.308  -4.732  1.00 35.05      S
ATOM   6096  OH2 TIP S 353       3.368  14.285  32.732  1.00 36.22      S
ATOM   6097  OH2 TIP S 354      -7.181  18.881 -31.723  1.00 38.24      S
ATOM   6098  OH2 TIP S 355     -28.089 -22.839 -28.744  1.00 37.10      S
ATOM   6099  OH2 TIP S 356      20.976  15.824 -10.665  1.00 30.49      S
ATOM   6100  OH2 TIP S 357     -28.758 -11.680 -18.762  1.00 30.24      S
ATOM   6101  OH2 TIP S 358       7.259  27.237  24.216  1.00 43.84      S
ATOM   6102  OH2 TIP S 359      -1.640  22.549  -9.537  1.00 31.98      S
ATOM   6103  OH2 TIP S 360      -4.918 -24.935 -15.685  1.00 38.37      S
ATOM   6104  OH2 TIP S 361       4.941  -2.575  16.309  1.00 33.12      S
ATOM   6105  OH2 TIP S 362       9.096 -17.304  13.805  1.00 34.53      S
ATOM   6106  OH2 TIP S 363      -5.045  -8.870  15.785  1.00 34.10      S
ATOM   6107  OH2 TIP S 364      17.874   2.521  14.615  1.00 31.53      S
ATOM   6108  OH2 TIP S 365     -10.159 -16.244 -28.446  1.00 34.86      S
ATOM   6109  OH2 TIP S 366       4.946   7.818 -15.134  1.00 36.25      S
ATOM   6110  OH2 TIP S 367      -6.685 -11.153  14.460  1.00 34.00      S
ATOM   6111  OH2 TIP S 368      14.487 -20.336  24.009  1.00 40.57      S
ATOM   6112  OH2 TIP S 369      -1.563   6.524 -45.958  1.00 34.28      S
ATOM   6113  OH2 TIP S 370       0.375   7.077  23.000  1.00 39.83      S
ATOM   6114  OH2 TIP S 371      17.591  31.139   0.347  1.00 42.33      S
ATOM   6115  OH2 TIP S 372     -16.867  13.392 -37.376  1.00 41.73      S
ATOM   6116  OH2 TIP S 373     -12.567   7.824 -44.159  1.00 41.23      S
ATOM   6117  OH2 TIP S 374      26.381  23.140 -10.721  1.00 31.69      S
ATOM   6118  OH2 TIP S 375       9.272  35.080   2.703  1.00 40.85      S
ATOM   6119  OH2 TIP S 376       9.264   3.347  41.197  1.00 40.96      S
ATOM   6120  OH2 TIP S 377      25.188  14.056  27.610  1.00 34.17      S
ATOM   6121  OH2 TIP S 378       5.411  -5.742  41.987  1.00 42.27      S
ATOM   6122  OH2 TIP S 379     -11.338  22.385 -17.862  1.00 32.59      S
ATOM   6123  OH2 TIP S 380     -20.579  13.226 -28.071  1.00 32.84      S
ATOM   6124  OH2 TIP S 381       8.683   9.553   3.945  1.00 34.93      S
ATOM   6125  OH2 TIP S 382       0.828  11.135 -13.934  1.00 42.23      S
ATOM   6126  OH2 TIP S 383     -21.600 -31.698 -19.564  1.00 38.49      S
ATOM   6127  OH2 TIP S 384      21.597  31.274  15.485  1.00 35.82      S
ATOM   6128  OH2 TIP S 385      12.268  35.903   4.587  1.00 31.57      S
ATOM   6129  OH2 TIP S 386     -10.826  21.324 -11.527  1.00 38.64      S
ATOM   6130  OH2 TIP S 387      20.994  17.489  -8.086  1.00 40.11      S
ATOM   6131  OH2 TIP S 388     -18.148  20.285 -26.433  1.00 31.64      S
ATOM   6132  OH2 TIP S 389      18.469  17.950  25.908  1.00 38.40      S
ATOM   6133  OH2 TIP S 390     -17.756   2.318 -44.136  1.00 37.68      S
ATOM   6134  OH2 TIP S 391      23.292  -5.751  18.962  1.00 37.56      S
ATOM   6135  OH2 TIP S 392      -5.798   2.354 -16.069  1.00 37.13      S
ATOM   6136  OH2 TIP S 393       2.260  -2.829 -24.110  1.00 34.35      S
ATOM   6137  OH2 TIP S 394      -1.341   7.648 -15.393  1.00 33.61      S
ATOM   6138  OH2 TIP S 395      14.575   6.039 -16.208  1.00 33.64      S
ATOM   6139  OH2 TIP S 396      21.269  15.381  -6.817  1.00 40.16      S
ATOM   6140  OH2 TIP S 397      11.903  28.956   0.420  1.00 35.70      S
ATOM   6141  OH2 TIP S 398       8.524 -21.963  24.816  1.00 30.69      S
ATOM   6142  OH2 TIP S 399     -19.214 -17.096  20.987  1.00 39.79      S
ATOM   6143  OH2 TIP S 400     -30.167 -21.541  -5.640  1.00 38.19      S
ATOM   6144  OH2 TIP S 401       9.901   9.176   7.979  1.00 37.49      S
ATOM   6145  OH2 TIP S 402      -4.981 -29.566  -1.767  1.00 34.27      S
ATOM   6146  OH2 TIP S 403      22.136  13.679  -1.917  1.00 36.13      S
ATOM   6147  OH2 TIP S 404     -13.420  -2.821  26.291  1.00 31.35      S
ATOM   6148  OH2 TIP S 405     -21.015 -10.324  -1.067  1.00 35.17      S
ATOM   6149  OH2 TIP S 406       4.107 -17.741  35.320  1.00 29.07      S
ATOM   6150  OH2 TIP S 407      20.599  24.525  23.153  1.00 39.40      S
ATOM   6151  OH2 TIP S 408     -29.430  -5.137 -24.706  1.00 31.71      S
ATOM   6152  OH2 TIP S 409       6.574  17.571  29.465  1.00 37.78      S
ATOM   6153  OH2 TIP S 410      25.806  21.628  -4.370  1.00 39.24      S
ATOM   6154  OH2 TIP S 411     -18.143 -31.597 -26.039  1.00 38.21      S
ATOM   6155  OH2 TIP S 412      -1.328  25.281 -12.054  1.00 31.58      S
ATOM   6156  OH2 TIP S 413       0.344  10.818  20.777  1.00 42.29      S
ATOM   6157  OH2 TIP S 414     -18.150 -29.804 -21.191  1.00 35.29      S
ATOM   6158  OH2 TIP S 415     -23.823  -3.528 -33.040  1.00 40.40      S
ATOM   6159  OH2 TIP S 416       1.739   1.943  19.314  1.00 36.07      S
ATOM   6160  OH2 TIP S 417     -27.131 -17.300 -23.592  1.00 38.57      S
ATOM   6161  OH2 TIP S 418      17.275   0.759  18.671  1.00 31.62      S
ATOM   6162  OH2 TIP S 419       0.007  26.223  -9.446  1.00 41.38      S
ATOM   6163  OH2 TIP S 420     -13.181 -10.416  10.475  1.00 37.29      S
ATOM   6164  OH2 TIP S 421     -18.110  16.629 -32.614  1.00 36.54      S
ATOM   6165  OH2 TIP S 422       7.358  26.526  17.628  1.00 39.18      S
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Figure 1 (continued 62)

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ATOM   6166  OH2 TIP S 423    17.448 -14.531  17.011  1.00 35.91       S
ATOM   6167  OH2 TIP S 424   -10.700 -26.518  31.162  1.00 35.06       S
ATOM   6168  OH2 TIP S 425    -9.328  -9.491  -8.639  1.00 37.90       S
ATOM   6169  OH2 TIP S 426   -17.105 -29.156 -14.203  1.00 24.63       S
ATOM   6170  OH2 TIP S 427     5.332  11.493  13.731  1.00 37.93       S
ATOM   6171  OH2 TIP S 428     6.050   9.224  14.792  1.00 30.75       S
ATOM   6172  OH2 TIP S 429     4.345  13.808  15.393  1.00 29.44       S
ATOM   6173  OH2 TIP S 430     8.193  12.380  12.091  1.00 21.45       S
ATOM   6174  OH2 TIP S 431   -28.556 -20.447 -15.197  1.00 37.37       S
ATOM   6175  OH2 TIP S 432    12.135  28.679  16.661  1.00 40.91       S
ATOM   6176  OH2 TIP S 433     6.265  25.002  25.462  1.00 33.19       S
ATOM   6177  OH2 TIP S 434    -2.131 -25.697  31.299  1.00 31.13       S
ATOM   6178  OH2 TIP S 435    -5.343 -20.243  26.687  1.00 32.69       S
ATOM   6179  OH2 TIP S 436   -24.850 -28.762  -6.570  1.00 37.97       S
ATOM   6180  OH2 TIP S 437   -22.436   0.184 -22.971  1.00 44.02       S
ATOM   6181  OH2 TIP S 438     1.275  22.882 -25.085  1.00 48.03       S
ATOM   6182  OH2 TIP S 439     7.058  13.884  -6.158  1.00 31.71       S
ATOM   6183  OH2 TIP S 440    13.032  24.424  22.464  1.00 39.78       S
ATOM   6184  OH2 TIP S 441    20.078  26.105  19.324  1.00 31.16       S
ATOM   6185  OH2 TIP S 442     4.931 -19.598  38.096  1.00 32.92       S
ATOM   6186  OH2 TIP S 443    -5.576 -22.456  27.255  1.00 65.54       S
ATOM   6187  OH2 TIP S 444    22.214  -2.644  27.541  1.00 35.37       S
ATOM   6188  OH2 TIP S 445    20.892   5.709  27.304  1.00 39.35       S
END
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Figure 1 (continued 63)
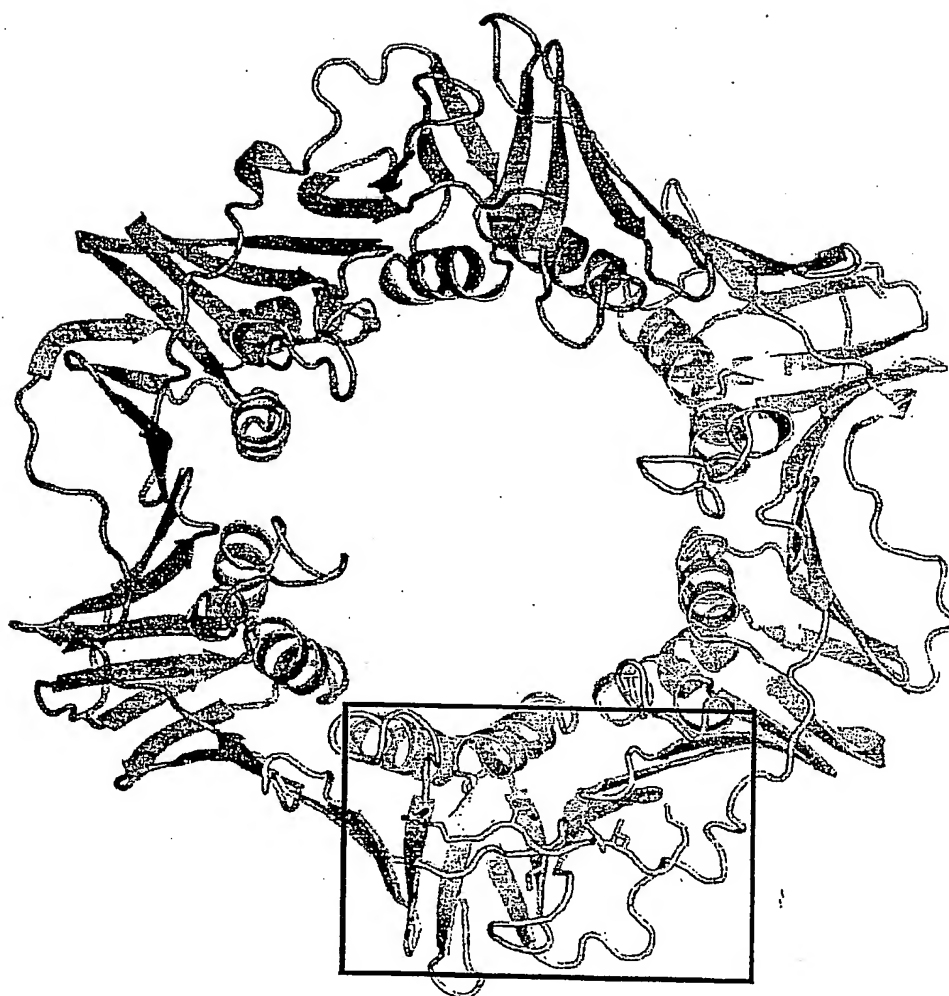
Figure 2
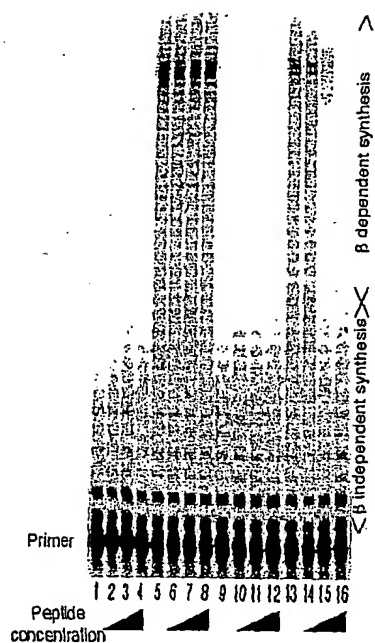
Figure 3A
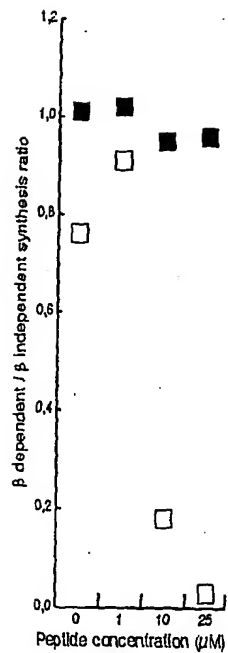
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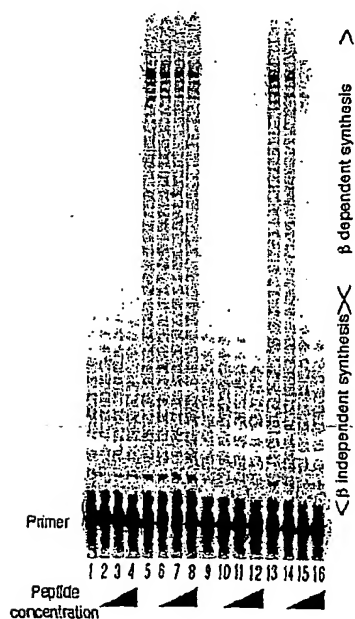
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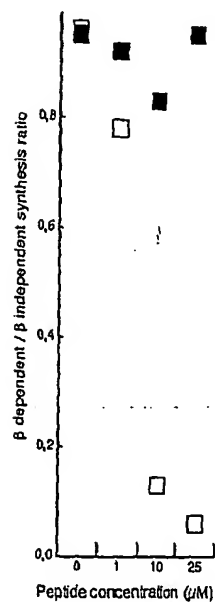
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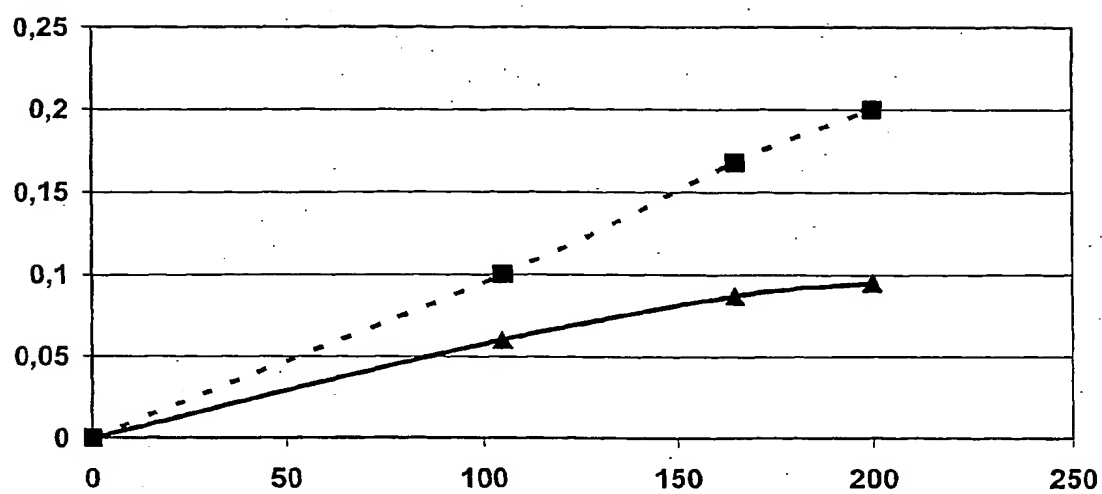
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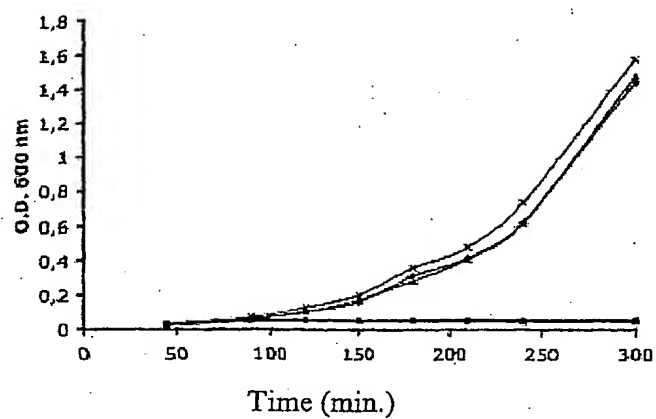
Figure 5A

Figure 5B

Figure 6